

Variational Principles and Cosmological Models in Higher-Order Gravity

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Doctoral dissertation

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*“O, for a Muse of fire, that would ascend
The brightest heavens of invention;
A kingdom for a stage, princes to act
And monarchs to behold the swelling scene!”*

— W. Shakespeare, Henry V, Prologue.

Preface

THIS doctoral dissertation is the fruit of five years of full-time research undertaken at the Department of Astrophysics and Geophysics of the University of Liège on January 1, 1994. Basically, it can be thought of as an extension of my MSc thesis, the scope of which was to present in a self-contained fashion the Hamiltonian formulation of a specific class of alternative, higher-order theories of gravity, namely those relativistic, metric theories based on quadratic curvature Lagrangians. In 1996 I had the opportunity to stay at the Department of Mathematics of the University of the Aegean for two months; the fruitful interplay with my Greek collaborators has undoubtedly broadened my research concerns in general relativity and cosmology and permeates a significant part of this doctoral dissertation.

When I started to work on alternative gravity theories, I planned to provide the reader of this yet unwritten dissertation with an exhaustive review of higher-order theories of gravity. However, I soon realised that the history of these theories is fairly intricate, hence quite difficult to summarise; an exhaustive account with a wide historical perspective would thereby be—very—lengthy and not suited to the present work. Still, I am deeply convinced that understanding the essential motivations of our predecessors greatly helps in finding one's path in scientific research; but this takes much time, thereby implying less published articles: This is not particularly welcomed according to modern standards. Fortunately, during the last five years I have never been put under pressure to submit a paper every three months or so.

I wish that the interested reader will find this dissertation helpful and pleasant to read ...

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Abstract

This dissertation investigates three main topics, all of which dealing with alternative, higher-order gravity theories in four dimensions. Firstly, we study the variational and conformal structure of those theories. Next, we analyse their Hamiltonian formulation and in particular its relationship with the famous ADM canonical version of general relativity. Finally, we study higher-order spatially homogeneous cosmologies and exemplify how Hamiltonian methods can be utilised to simplify the analysis of the associated field equations.

As regards the first topic, we begin by critically reviewing the variational principle in gravitational theory: We argue that the ‘Einstein–Palatini’, metric-affine method of variation, aside from being inherently nonequivalent to the Hilbert, purely metric variational principle, leads to inconsistencies when applied to generalised gravitational actions including higher-order curvature terms. This conveys us to put forth that one possible scheme that does not exhibit the cumbersome features of the ‘Einstein–Palatini device’ is the Lagrange-multiplier version of the latter, namely the constrained first-order formalism. Applying this constrained method of variation to a general class of nonlinear Lagrangians we prove that the conformal equivalence theorem of these nonlinear theories with general relativity and an additional scalar field holds in the extended framework of Weyl geometry. As a direct consequence, we demonstrate that the Einstein–Palatini method is a degenerate case of the constrained first-order formalism and that it is unable to deal with Weyl spaces. This investigation sheds another light on what is sometimes referred to as the *universality of Einstein’s equations*.

Next, we give a detailed account of the Hamiltonian formulation of higher-order gravity theories. After a short summary of Dirac’s formalism for constrained systems, we thoroughly analyse the procedure that enables one to develop a consistent canonical formulation of any field theory involving higher derivatives: the generalised Ostrogradsky method. We demonstrate the effectiveness of this *modus operandi* by expressing nonlinear gravitational Lagrangians in canonical form. This conveys us to the main result in this part, that is, the equivalence of the Ostrogradsky and ADM canonical versions of general relativity. We then discuss the issue of boundary terms in the light of the Ostrogradsky formalism. We finally obtain the explicit forms of the Hamiltonian constraints and canonical equations derived from generic quadratic Lagrangians.

The last topic is devoted to the study of spatially homogeneous Bianchi-type cosmologies in higher-order gravity. We firstly analyse the empty Bianchi-type IX or *mixmaster* model in the full fourth-order gravity theory—without resorting to the Ostrogradsky scheme—on approach to the initial singularity; we prove that the mixmaster chaotic behaviour based on the BKL piecewise approximation method is structurally unstable and that there exists an isotropic power-law solution reaching the initial singularity in a stable, monotonic way. Next, we particularise the aforementioned Ostrogradsky canonical formalism to class A Bianchi types in the two distinct variants of the generic quadratic theory, namely the pure ‘ R -squared’ case and the conformally invariant, ‘Weyl-squared’ case respectively. In the former we reduce the system of canonical equations to a system of autonomous second-order coupled differential equations that we solve analytically for Bianchi type I. In the latter we prove that the Bianchi-type I system is not integrable—in the sense of Painlevé—; we determine all particular closed-form solutions and discuss their conformal relationship with Einstein spaces.

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Sommaire

Dans cette thèse, nous étudions divers aspects liés aux théories alternatives de la gravitation contenant des termes d'ordre supérieur en la courbure, dans des espaces-temps à quatre dimensions. Nous analysons successivement la structure variationnelle et conforme de ces théories ainsi que leur formulation hamiltonienne. Ensuite, nous procédons à l'étude de modèles spatialement homogènes et, en particulier, nous montrons comment le formalisme canonique peut conduire à une simplification dans la recherche de solutions exactes.

Dans la première partie, après avoir insisté sur le fait que le principe variationnel d'Einstein-Palatini n'est, en général, pas équivalent au principe de Hilbert et qu'il présente des incohérences manifestes dès qu'il est appliqué à des théories autres que la relativité générale dans le vide, nous avançons qu'un schéma consistant ne souffrant pas de ces difficultés est fourni par la méthode de variation métrique-affine avec multiplicateurs de Lagrange. Nous démontrons que l'équivalence conforme des théories non linéaires de la gravitation avec la relativité générale et un champ scalaire additionnel est également vérifiée dans le cadre géométrique étendu des espaces de Weyl. Comme corollaire, nous prouvons que la méthode d'Einstein-Palatini est un cas dégénéré du formalisme avec contraintes et qu'elle ne permet pas de travailler en géométrie de Weyl. Sous cet angle, nous donnons une interprétation différente de ce qui est appelé, dans la littérature récente, *universalité des équations d'Einstein*.

Nous analysons ensuite de façon détaillée la formulation hamiltonienne des théories de la gravitation d'ordre supérieur. Après avoir rappelé les ingrédients nécessaires à une telle construction, c'est-à-dire le formalisme de Dirac des systèmes contraints et la méthode d'Ostrogradsky généralisée, nous illustrons l'efficacité de cette dernière en construisant explicitement une formulation canonique des théories à lagrangiens non linéaires en la courbure. Considérant le lagrangien d'Einstein-Hilbert comme cas particulier, nous démontrons le résultat majeur de cette partie, à savoir l'équivalence entre la formulation d'Ostrogradsky de la relativité générale et le célèbre formalisme ADM. Sous ce nouvel éclairage, nous discutons ensuite le problème des termes de surface pour les théories d'ordre supérieur. Enfin, nous obtenons la forme explicite des contraintes et des équations canoniques provenant du lagrangien quadratique le plus général.

La dernière partie du travail est consacrée à l'étude de modèles spatialement homogènes dans le cadre des théories quadratiques de la gravitation. Tout d'abord, nous montrons que, au voisinage de la singularité initiale, le comportement oscillatoire et chaotique du modèle anisotrope Bianchi IX basé sur l'approximation dite de BKL est structurellement instable pour la théorie générale purement quadratique. Ensuite, nous particularisons le formalisme canonique d'Ostrogradsky aux modèles de Bianchi de classe A, en distinguant les deux variantes significatives de la théorie quadratique générale, à savoir, le cas où le lagrangien se réduit au carré de la courbure scalaire et le cas conformément invariant, où le lagrangien est égal au produit quadratique contracté du tenseur de Weyl. Dans la première variante, nous réduisons le système canonique de départ à un système d'équations différentielles autonomes du second-ordre que nous résolvons analytiquement pour Bianchi I. Dans la seconde, pour ce même modèle, nous démontrons que le système canonique n'est pas intégrable, au sens de Painlevé, nous déterminons toutes les solutions analytiques particulières et discutons leur relation conforme avec des espaces d'Einstein.

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Chapter 1

Introduction

*“By Him who gave to our soul the Tetraktys, which hath
the fountain and root of ever-springing nature.”*

— Pythagorean’s oath.

NOTWITHSTANDING the fact that Einstein’s general relativity is experimentally tested with an overwhelmingly high degree of accuracy—from solar system tests to binary pulsars observational data—, it has become a peremptory necessity to consider *alternative* theories of gravity. The reasons can be summarised as follows. Firstly, although Einstein’s theory is the simplest—and the most aesthetic—geometrical theory of gravitation settled on the basic postulates of the *equivalence principle* and *general covariance* of the physical laws, there are no a priori reasons whatsoever to restrict the gravitational Lagrangian to be a *linear* function of the scalar curvature nor to discard other more complicated frameworks obtained upon suitable generalisations of the Einstein–Hilbert Lagrangian of general relativity. Examples of such extensions are: scalar-tensor theories and higher-order gravity theories in four dimensions; Kaluza–Klein multidimensional theories; gauge theories of gravity, with torsion and ‘non-metricity’. Secondly, a strong research effort has been produced so far in different directions in order to formulate a consistent quantum theory of gravity; although the electroweak and strong interactions are described by renormalisable quantum field theories, Einstein’s gravitational theory cannot be quantised according to the standard schemes, for the Einstein–Hilbert action (with possibly a cosmological constant Λ)

$$S_{\text{EH}} = \int d^4x \sqrt{-g} \frac{c^3}{16\pi G_{\text{N}}} (R - 2\Lambda)$$

does not define a renormalisable quantum field theory. However, by adding to this action the most general, covariant action that contains quadratic curvature terms

and dimensionless couplings, namely

$$S_* = \int d^4x \sqrt{-g} (\alpha R^2 - \beta C^2 + \gamma L_{\text{GB}} + \delta \square R),$$

where C^2 denotes the contracted quadratic product of the Weyl tensor, L_{GB} the Gauss–Bonnet term (topological invariant), and the ‘box’ the d’Alembertian differential operator,¹ one obtains a power-counting renormalisable theory [UD62],² which is asymptotically free [FT81]. Secondly, one hopes that such alternative theories might provide one with a better approximation, semi-classical limit of a yet unknown quantum theory of gravity. Amongst the various attempts to understand what a quantum space-time really is, unifying schemes such as string theory, supergravity, or more generally M-theory play a prominent rôle (see, e.g., [Rov98, Gib98] for very recent reviews); and it turns out that higher-derivative terms appear naturally in the low-energy effective Lagrangians of some of those theories. Thirdly, the standard model of relativistic cosmology suffers from a certain number of difficulties that could perhaps be more naturally resolved in the context of generalised theories. For instance, whereas the singularity theorems in general relativity show that the occurrence of space-time singularities is a generic feature of any cosmological models (under some reasonable conditions), it might happen that in the context of alternative theories those unwanted singularities could be avoided; in fact, during the last decade the absence of cosmological singularities when higher-order curvature terms are taken into account has been pointed out in the literature several times (see, e.g., [KRT98] and references therein).

As stated in the Preface, we do not intend to give an historical perspective of the development of higher-order theories of gravity. We just would like to mention that it can be traced back to the early years of general relativity, when great physicists like Weyl, Einstein, Bach, and others were undertaking the first investigations aiming at modifying the Hilbert variational principle so as to unify—on purely geometrical grounds—electromagnetic and gravitational phenomena. Although this programme proved to be, so to speak, ‘chimeric’, it gave a renewed insight into the powerful use of the variational principle in gravitational theory and led many researchers to extend its domain of applicability to for instance other geometries or greater dimensions. Nowadays, the geometrical structure of any theory is intimately connected with its formulation in terms of an action, in Lagrangian or Hamiltonian form, from which are derived the field equations by means of a specific, properly defined variational principle. Because of the proliferation of various

¹For a list of the conventions and notations used throughout this dissertation, cf. page 6.

²Rigorous renormalisability of the general fourth-order action has been proved by Stelle using BRS invariance [Ste77].

types of alternative gravity theories, it is of fundamental importance not just to confront their theoretical predictions with observational data but also to expressly understand their geometrical structure and the possible interconnections between their respective solution spaces. For instance, one question worth to be addressed in that respect is whether the conformal equivalence between a certain class of alternative theories and general relativity would hold in the context of metric-affine variations of generalised actions in Weyl geometry; another is to analyse the Hamiltonian formulation of those theories and possibly their quantisation. As regards higher-order theories though, it should be borne in mind that the field equations are much more intricate than Einstein's—any method of order reduction is thus most welcomed.

Whereas plane wave solutions of linearised Einstein gravity propagate two physical degrees of freedom, carrying helicity ± 2 , the most general quadratic gravitational Lagrangian has eight degrees of freedom: a massless spin-2 state, a massive spin-0 state, and a massive spin-2 ghost [Ste77, Ste78]. Higher-order gravity theories have not received general acceptance *as viable physical theories* because some solutions of the classical theory are expected to have no lower energy bound and therefore exhibit instabilities, namely ‘runaway solutions’: the linearised field equations propagate ghosts, i.e. negative-energy modes, and possibly tachyons.³ However, crucial *nonperturbative* results have changed the bad reputation associated with this nonunitary character. For instance, the *zero-energy theorem* states that: Although the theory admits linearised solutions with negative energy all exact solutions representing isolated (asymptotically flat) systems have precisely zero energy; the solutions to the linearised equations with nonzero energy of either sign do not correspond to the limit of a one-parameter family of exact solutions [BHS83]. An interesting consequence of this theorem is that one cannot draw conclusions from the linearised theory concerning the stability of the full quantum theory.

One special variant of the generic quadratic theory, which has attracted much interest as a promising candidate for quantum gravity, is called *conformal gravity*;⁴ it is the purely quadratic theory based on an action containing only the Weyl-squared, C^2 term, which possesses the aesthetically pleasing feature of being the local gauge theory of the conformal group and hence locally scale invariant. This means that the theory bears no resemblance to Einstein gravity classically; it encompasses six degrees of freedom corresponding to massless spin-2 and spin-1 ordinary states and a massless spin-2 ghost state [LN82, Rie84]. Conformal gravity satisfies at least two remarkable properties [Rie86]: Birkhoff's theorem holds—in

³This drawback of higher-order gravity pertains in fact to any theory with higher derivatives; see, e.g., [PU50].

⁴For a detailed bibliography, the interested reader may consult [Que98].

stark contrast to the generic quadratic case—and nonperturbative effects can confine the ghosts—analogously to the confinement of colour in quantum chromodynamics. The conformal fourth-order field equations, first put forth by Bach [Bac21], are found in differential geometry and in mathematical studies of Einstein’s field equations of general relativity that use conformal techniques; they also constitute necessary conditions for a space to be conformal to an Einstein space. The classical study of the Bach equations is partly justified by the fact that conformal gravity has been viewed, during the last decade, as a possible, physically viable alternative theory of gravity that would be able to resolve some of the problems general relativity alone is unable to address without ad hoc assumptions such as, for instance, the dark matter hypothesis [MK89]. However, a deeper investigation reveals other open problems that necessitate further consideration (see, e.g., [Kle98] for the most recent contribution). In particular, little work has been done in regard to spatially homogeneous cosmologies.

Aside from conformal gravity, it is of great interest to study other variants of higher-order theories in the context of cosmology. The Friedmann–Lemaître–Robertson–Walker (FLRW) spaces, which are isotropic and are homogeneous on spacelike sections, constitute the basic pillar of the standard model of cosmology, which successfully accounts for many of the observed features of our universe. However, this scheme is not free from certain riddles: the so-called ‘horizon’, ‘flatness’, and ‘smoothness’ problems. These are addressed, more or less adequately, by incorporating the generally accepted inflationary paradigm into the orthodox isotropic cosmology with additional ingredients such as hot and cold dark matter blends—Is anybody still laughing at Ptolemaic epicycles? It is known that generalised gravity theories such as quadratic or scalar-tensor theories do possess solutions exhibiting an inflationary stage; in addition, they could possibly provide us with more satisfactory mechanisms to trigger inflation. On the other hand, mathematical cosmology focusses more on spatially homogeneous and *anisotropic* models since they are fairly more general than the FLRW universes and because one aims to investigate specific issues, such as for instance the genericness of oscillatory, chaotic dynamical regimes on approach towards the initial singularity, unhindered by the stringent symmetry requirement that the universe be isotropic *ab initio*.

In this dissertation we examine Lagrangian and Hamiltonian variational methods for higher-order gravitational actions and in particular for nonlinear and conformally invariant theories; we apply these methods to study the classical solution space of spatially homogeneous cosmological models in higher-order gravity. The outline is the following:⁵

⁵A more detailed plan is provided at the beginning of each of those chapters, i.e. on pp. 9, 49, and 125 respectively.

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- In Chapter Two we begin by critically reviewing the variational principle in gravitational theory; we analyse the metric-affine variational method in the context of generalised gravity theories in order to seek in which specific circumstances it can be utilised to deal with extended geometrical settings, such as Weyl geometry. We show that the Einstein–Palatini method exhibits inconsistencies and that it is a degenerate case of the constrained first-order formalism, which is the appropriate framework that can incorporate general Weyl spaces. We prove the chief result of this chapter, namely that the conformal equivalence theorem of nonlinear theories with general relativity and additional scalar fields holds in the extended framework of Weyl geometry. As a direct consequence, we give a different interpretation of a universality property of Einstein’s equations found in the context of the Einstein–Palatini method.
 - In Chapter Three we focus on the Hamiltonian formulation of theories with higher derivatives. After a short summary of Dirac’s formalism for constrained systems and a detailed account of the generalised Ostrogradsky method, we develop a canonical formulation of nonlinear gravitational Lagrangians of the type $f(R)$. Next, we prove the most important result of this chapter, namely that the Ostrogradsky Hamiltonian formulation of general relativity is equivalent to its well known ADM canonical version. We then discuss the issue of boundary terms in the light of the Ostrogradsky formalism and give the explicit forms of the super-Hamiltonian and super-momentum constraints, and of the canonical equations that are derived from generic quadratic Lagrangians.
 - In Chapter Four we study spatially homogeneous Bianchi-type cosmological models in some variants of higher-order gravity. We firstly analyse the empty Bianchi-type IX or mixmaster model in the purely quadratic theory—without resorting to the Ostrogradsky method—on approach to the initial singularity; we prove that the mixmaster chaotic behaviour based on the BKL approximation scheme is structurally unstable and that there exists an isotropic power-law solution reaching the initial singularity in a stable, monotonic way. Next, we particularise the results obtained at the end of Chapter Three to class A Bianchi types in the two distinct variants of the generic quadratic theory, namely the pure ‘ R -squared’ case and the conformally invariant, ‘Weyl-squared’ case respectively. In the former we reduce the system of canonical equations to a system of autonomous second-order coupled differential equations that we solve analytically for Bianchi type I. In the latter we prove that the Bianchi-type I system is not integrable—in the sense of

Painlevé—; we determine all particular solutions that may be written in closed analytical form and discuss their conformal relationship with Einstein spaces.

Conventions and notations

In this dissertation we adopt the sign conventions of the gravitation bible [MTW73]; in particular we use the metric signature $(-+++)$. We also make use of a ‘customised version’ of the *abstract index notation* discussed in [Wal84]: Latin indices of a tensor that belong to the beginning of the alphabet a, b, c, \dots denote the type of the tensor—not its components—; Latin indices of a tensor that belong to the middle of the alphabet i, j, k, \dots refer to spacelike components in the Cauchy hypersurfaces Σ_t defined by the slicing of space-time; however, in Chapter 2 we do not employ Greek indices $\alpha, \beta, \gamma, \dots$ to refer to the components of a tensor with respect to a specific coordinate space-time basis: we keep Latin indices a, b, c, \dots instead.

The symbol ∇_a usually stands for the covariant derivative operator but occasionally denotes the associated linear affine connection. In Chapter 2 we also employ the symbol $\overset{\circ}{\nabla}_a$ to refer to the covariant derivative operator associated with the Levi-Civita connection, the components of which in a non-coordinate basis are

$$\Gamma^\mu_{\alpha\beta} = \left\{ \begin{smallmatrix} \mu \\ \alpha\beta \end{smallmatrix} \right\} + \frac{1}{2}g^{\mu\nu}(C_{\beta\nu\alpha} + C_{\alpha\nu\beta} - C_{\nu\alpha\beta}),$$

where $\left\{ \begin{smallmatrix} \gamma \\ \alpha\beta \end{smallmatrix} \right\}$ are the Christoffel symbols, i.e. the components of the Levi-Civita connection in a natural basis, and the C ’s are the structure coefficients of the non-coordinate basis.

The Riemann curvature tensor is defined by

$$\begin{aligned} R^a_{bcd} u^b &= (\nabla_c \nabla_d - \nabla_d \nabla_c) u^a, \\ R_{cdb}{}^a v_a &= -R^a_{bcd} v_a = (\nabla_c \nabla_d - \nabla_d \nabla_c) v_b, \end{aligned}$$

for arbitrary vectors u^b and one-forms v_a , where ∇_a is the covariant derivative operator. The Ricci tensor is obtained by contraction on the first and third indices, that is

$$R_{ab} = R^c_{acb}.$$

Gothic characters denote tensor densities; e.g., $\mathfrak{A}^{ab} := \sqrt{-g} A^{ab}$; round and square brackets around indices denote respectively symmetrisation and antisymmetrisation (including division by the number of permutations of the indices); a tilde denotes conformally transformed quantities.

Unless otherwise stated we use *geometrised units*, where the Newton gravitational constant G_N and the speed of light in vacuum c are set equal to one: $G_N = 1 = c$.

We adopt Schouten's nomenclature for the type of spaces considered [Sch54]. An L_n is a general n -dimensional manifold endowed with a *linear* connection; when the latter is *symmetric* the L_n is called an A_n and is torsion-free. When a metric tensor g_{ab} is defined, the compatibility condition does not hold in general, i.e. $\nabla_c g_{ab} = -Q_{cab} \neq 0$. If $Q_{cab} = 0$, the connection is called *metric* with respect to g_{ab} and the L_n is called a U_n ; if in addition the connection is symmetric, one has a V_n , i.e. *Riemann space*. If $Q_{cab} = Q_c g_{ab}$, the connection is called *semi-metric*; if in addition it is symmetric, the L_n is called a W_n , i.e. *Weyl space*.

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Chapter 2

Variational and conformal structure in higher-order gravity

“Sub fide vel spe geometricantis naturæ.”

— Giordano Bruno.

VARIATIONAL PRINCIPLES play a prominent rôle in theoretical physics; it has become well accepted during this century that any fundamental physical theory can be formulated in terms of an action, in Lagrangian or Hamiltonian form, from which are derived the equations of motion by means of a variational principle. For the last decades this has been raised to a metalaw of nature: Nowadays, setting up a (field) theory means that one starts to write an action in terms of the fields one considers, even if the knowledge of the actual form of their interactions and symmetry properties is fragmentary. Specification of the Lagrangian function is determined by mathematical and physical requirements like gauge invariance, renormalisability, simplicity, and so forth. Yet, certain peculiarities of the Lagrangian that arise under symmetry transformations, such as the appearance of a total divergence, might indicate “that one is dealing with some approximation or a limiting case of a ‘better’ theory, in which the corresponding, possibly modified, symmetries fully preserve the action integral” [Tra96].

Even though we do not intend to discuss epistemological or metaphysical issues related to the significance of the variational method we would like to emphasise that, historically, it has often been the focus of philosophical contentions and misconceptions for, in contradiction to the usual *causal* description of phenomena, “the idea of enlarging reality by including ‘tentative’ possibilities and then selecting one of these by the condition that it minimizes a certain quantity, seems to bring a *purpose* to the flow of natural events” [Lan49, p. xxiii]. Still, one ought not be

disconcerted: For the universal mind of the seventeenth and eighteenth centuries, the two ways of thinking did not necessarily appear contradictory. Leibniz who had a strong influence on the development of the variational method—for example, the present use of the word ‘action’ in physics probably originates from Leibniz’s expression *actio formalis*—had strong teleological propensities, which also characterised the ideas of Fermat, Borelli, and Maupertuis. By contrast, the sober, matter-of-fact nineteenth century—which still gets hold of numerous present-day scientists—looked at the variational principles (of mechanics) merely as convenient alternative mathematical formulations of the fundamental laws, without any primary importance whatsoever. This pragmatic point of view has however changed with the advent of general relativity—in the light of which “the application of the calculus of variations to the laws of nature assumes more than accidental significance” [Lan49]—and quantum mechanics—especially with regard to Feynman’s ‘sum-over-histories’ approach, in relation with Dirac’s deep intuition [FH65, MTW73].¹

As stated in the Introduction, we aim to analyse the metric-affine variational method as applied to gravity theories in order to determine in which specific circumstances it can be regarded as a possible generalisation of the standard metric variational principle of general relativity. First of all, we make a brief historical survey to see how the metric-affine variational principle was introduced in general relativity.²

The *purely metric* or Hilbert variational principle of general relativity was properly defined during the years 1914 to 1916 owing to the works of Einstein, Hilbert, and Lorentz for any of whom, at that time, the metric tensor was thought of as the only fundamental gravitational field. However, from the early works of Levi-Civita and Hessenberg in 1917, Weyl and Cartan developed, until 1923, the new concept of affine connection on manifolds without a metric structure. For many years Weyl’s theory of symmetric linear connections [Wey50a] has been a rich source of inspiration for himself and physicists like Eddington and Einstein whose aim was to unify—on purely geometrical grounds—gravitational and electromagnetic phenomena by means of an *affine* variational principle. Unfortunately their attempts did not meet their hopes and Einstein abandoned the purely affine theory on behalf of a *metric-affine* variational method in which the metric tensor and the affine connection are considered as independent fields through the process of variation; Einstein proved exactly, for the first time, what is placed in most modern textbooks under the authorship of Palatini—even though Palatini’s contribution (cf. equation

¹In particular, we now know that the *value* of the action integral—and not only its *variation*—is physically relevant.

²For a more detailed account, we refer the interested reader to [FFR82, Viz89, Que98], and references therein.

(2.7)) was formulated in a purely metric framework [Pal19, Pau58]—, namely the equivalence of Einstein’s field equations of vacuum general relativity and the field equations that are derived by means of metric-affine independent variation of the Einstein–Hilbert gravitational action [Ein25]. Once again, Einstein’s attempt of a geometric unification failed and the metric-affine method lost its interest—even if Schrödinger revisited the question twenty years later [Sch50]—until the late fifties with the works of Stephenson [Ste58, Ste59] and Higgs [Hig59] who analysed the field equations obtained from quadratic Lagrangians via a metric-affine variational principle; more specifically, they considered those equations as an alternative set to Einstein’s field equations: The choice of Lagrangians—quadratic in the various curvature tensors—was again motivated by Weyl’s unified theory of gravitation and electromagnetism.³ However, Buchdahl raised severe conceptual objections in regard to the self-consistency of the method and proposed implicitly to abandon the use of ‘Palatini’s device’ in gravitational theory [Buc60].

At the same time the so-called ‘Hilbert–Palatini action principle’ together with the ‘three-plus-one decomposition’ of space-time was invoked successfully by Arnowitt, Deser, and Misner (ADM) in order to develop a Hamiltonian formulation of general relativity [ADM62, MTW73, §21.2 and §21.7].⁴ However, referring to the ‘Palatini variational principle’ is misleading. As a matter of fact, there is no need whatsoever to resort to a metric-affine variation in order to rewrite the Einstein–Hilbert action in canonical form.⁵ In that respect, the analogy (cf. [MTW73, §21.2]) between the ‘Palatini variation’ and Hamilton’s principle in phase space is inaccurate—*stricto sensu* it is wrong.⁶ In fact, the conjugate momenta are defined in terms of the extrinsic curvature, not in terms of the connection; the equivalence of purely metric and metric-affine variations in *vacuum* general relativity is a mere coincidence (cf. Subsection 2.1.2).

In the same spirit as in Stephenson’s articles, Yang investigated a theory based on a Lagrangian that is quadratic in the Riemann tensor, by analogy with the Yang–

³There were numerous attempts towards that goal, which were chiefly characterised by a modification of the variational principle through different kinds of alteration of its underlined geometric structure: semi-Riemannian manifolds in dimensions greater than four (e.g., Kaluza–Klein theories); nonmetric connections (e.g., Weyl geometry, theories with torsion); purely affine connections (e.g., Einstein–Schrödinger theory); and so forth. For an exhaustive study on all these alternative theories, we refer to the remarkable treatise of Tonnelat [Ton65].

⁴See Subsection 3.1.1 on page 50 and Subsection 3.3.1 on page 89.

⁵By contrast, the Ashtekar canonical formalism uses explicitly the Hilbert–Palatini first-order variational method, with the tetrad field and spin-connection as independent variables, and where only the self-dual part of the curvature is retained in the Lagrangian; see, e.g., [Pel94].

⁶This was clearly emphasised by El-Kholy, Sexl, and Urbantke who distinguished between what they called the ‘Palatini principle’ and the ‘formal Palatini method of variation’; the ADM procedure belonging to the second class [ESU73].

Mills Lagrangian [Yan74]. Unfortunately, Stephenson’s and Yang’s field equations are tainted by a conceptual mistake occurring in the process of variation. Before this error was noticed, several authors proved that those equations were leading to generic unphysical solutions and consequently they ruled them out.⁷

Extending previous results—only valid in vacuum general relativity—of Lanczos [Lan57] and Ray [Ray75], Safko and Elston applied the metric-affine variational principle with Lagrange multipliers to quadratic Lagrangians [SE76].⁸ Unacquainted with the Ostrogradsky method, they also tried to establish a connection between the Lagrange-multiplier version of the variational principle and the ADM formalism in order to develop a Hamiltonian formulation of quadratic gravity theories (cf. Subsection 3.3.4). Independently, Kopczyński showed that the introduction of appropriate constraints into the gravitational action may serve to ‘unify’ the variational derivations of distinct theories of gravity such as Einstein’s theory and the Einstein–Cartan theory [Kop75]. The most recent generalisations of this constrained method of variation, for manifolds with torsion and ‘non-metricity’, lead to the *metric-affine gauge theory of gravity* (MAG) [HMMN95].

Following Buchdahl [Buc79], we address the questions of the utility and consistency of this method of variation in the broader context of generalised gravity theories.⁹ More specifically, in Section 2.1 we briefly present the well-known Hilbert method of variation, mainly to settle our notations, and critically review the Einstein–Palatini variational principle in general relativity. In Section 2.2 we extend the study of the variational principle to the domain of higher-order Lagrangians; the ensuing picture reveals that the Einstein–Palatini variational principle is generically unreliable, already at the classical level. This conclusion conveys us to carefully formulate a Lagrange-multiplier version of the metric-affine variational method that we call *constrained first-order formalism*. As a first application, we consider the variation of several higher-order Lagrangians with a Riemannian constraint and correct Safko and Elston’s results [SE76]. Furthermore, we show that the equivalence of the field equations that are derived from appropriate actions via this formalism to those produced by variation of purely metric Lagrangians is not merely formal but is implied by the diffeomorphism covariant property of the associated Lagrangians. In Section 2.3, after a brief account of the conformal relationship between nonlinear and scalar-tensor gravitational Lagrangians and general relativity with additional scalar fields, we analyse the conformal structure of non-

⁷Notwithstanding this fact, a detailed study of Yang’s equations has been published most recently [GN98].

⁸In spite of several misprints in the resulting formulæ Safko and Elston’s conclusions are right; cf. Subsection 2.2.3.

⁹We restrict ourselves to geometries without torsion, i.e. symmetric connections.

linear gravity theories in the context of the constrained first-order formalism; in particular, we prove that the conformal equivalence theorem of those theories with general relativity plus a scalar field holds in the extended framework of Weyl geometry. This investigation enables us to give a different interpretation of what has been recently called a ‘universality property of Einstein’s equations’ [FFV94, BFFV98] and to invalidate a recent claim on a possible explanation of a—controversial—observed anisotropy in the universe [TU98, QMC99]. Finally, we point out how these results may be further exploited and address a number of new issues that arise from this analysis. This work was carried out in collaboration with S. Cotsakis and J. Miritzis [CMQ97] (see also [Mir97, Cot97, Que97]).

2.1 Variational principles in general relativity

2.1.1 Hilbert variation

Consider a four-dimensional space-time manifold \mathcal{M} endowed with a Lorentzian metric g_{ab} and assume that the connection ∇_c be the symmetric Levi-Civita connection, i.e. $\nabla_c g_{ab} = 0$; hence $(\mathcal{M}, \mathbf{g}, \nabla)$ is a V_4 , i.e. a Riemannian space. In the Lagrangian formulation of the theory the Hilbert metric variational principle proceeds with the specification of a Lagrangian density \mathfrak{L} , which is assumed to be a functional of the metric and its first and possibly higher derivatives, that is

$$\mathfrak{L} = \mathfrak{L}(\mathbf{g}, \partial \mathbf{g}, \partial^2 \mathbf{g}, \dots). \quad (2.1)$$

In addition, one requires that \mathfrak{L} be a scalar density of weight +1, i.e. $\mathfrak{L} = \sqrt{-g} L$, where g denotes the determinant of the matrix formed with the components of g_{ab} and L is the Lagrangian; this enables one to form the action integral

$$S[\mathbf{g}] = \int_{\mathcal{U}} d^4\Omega \mathfrak{L}, \quad (2.2)$$

where $d^4\Omega = dx^0 \wedge dx^1 \wedge dx^2 \wedge dx^3$, which is taken over a compact region \mathcal{U} of the manifold \mathcal{M} . The field equations are obtained by requiring that the action (2.2) be stationary under arbitrary variations such that the metric and its first derivatives be held fixed on the boundary $\partial\mathcal{U}$. This variation defines the functional derivative \mathfrak{L}_{ab} of the Lagrangian density \mathfrak{L} , viz.

$$\delta S[\mathbf{g}] = \int_{\mathcal{U}} d^4\Omega \mathfrak{L}_{ab} \delta g^{ab}, \quad \text{with } \mathfrak{L}_{ab} := \frac{\delta \mathfrak{L}}{\delta g^{ab}},$$

also called the *Euler-Lagrange derivative* of \mathfrak{L} , and the field equations are

$$\mathfrak{L}_{ab} = 0.$$

As is well known, the variational principle implies very important differential constraints on the field equations, which hold ‘off shell’, i.e. whether or not the field equations are satisfied; these are the *generalised Bianchi identities*, obtained from Noether’s second theorem by taking as a specific class of variations of the metric that induced by diffeomorphisms $f : \mathcal{M} \rightarrow \mathcal{M}$. Since the manifolds $(\mathcal{M}, \mathbf{g})$ and $(\mathcal{M}, f^*\mathbf{g})$ are physically equivalent, the action functional does not change under the diffeomorphism f ; in particular, it remains unaltered under an infinitesimal coordinate transformation. For such variations, it is not difficult to see that, at the first order of perturbation, δg^{ab} is given in terms of the Lie derivative of the metric with respect to the vector field v^c that generates the diffeomorphism f , that is,¹⁰

$$\delta g^{ab} = -\mathcal{L}_v g^{ab} = -2\nabla^{(a} v^{b)}.$$

Since by definition \mathfrak{L}_{ab} is a symmetric density of weight +1, the variational principle yields

$$\delta S[\mathbf{g}] = -2 \int_{\mathcal{U}} d^4\Omega \mathfrak{L}_{ab} (\nabla^a v^b) \equiv 0$$

for all vector fields v^c that vanish on the boundary. Integrating by parts the last equation and dropping the divergence term one obtains the expected generalised Bianchi identities, namely

$$\nabla^a \mathfrak{L}_{ab} = 0. \quad (2.3)$$

The simplest Lagrangian density for gravity is the Einstein–Hilbert Lagrangian density $\mathfrak{L}_{\text{EH}} = \sqrt{-g} R$, where $R = g_{ab} R^{ab}$ is the scalar curvature, to which one may possibly add a cosmological constant term $\Lambda\sqrt{-g}$. The corresponding gravitational action is

$$S = \frac{c}{2\kappa^2} \int_{\mathcal{U}} d^4\Omega \mathfrak{L}_{\text{EH}}, \quad (2.4)$$

where $\kappa^2 = 8\pi G_{\text{N}} c^{-2}$ is the Einstein gravitational constant.¹¹ The Ricci tensor R_{ab} is expressed in terms of the connection coefficients Γ^c_{ab} and their first derivatives, viz.

$$R_{ab} := R^c_{acb} = \partial_c \Gamma^c_{ab} - \partial_b \Gamma^c_{ac} + \Gamma^c_{cd} \Gamma^d_{ab} - \Gamma^c_{bd} \Gamma^d_{ac}.$$

¹⁰See [Wal84, Appendix C].

¹¹Hereafter we use ‘geometrised units’, where the Newton gravitational constant G_{N} and the speed of light in vacuum c are set equal to one, and we rescale the coordinates to absorb the constant factor 8π .

Since the ‘metricity’ or compatibility condition holds, i.e. $\nabla \mathbf{g} = 0$, the Γ ’s are the Christoffel symbols, namely

$$\Gamma^c_{ab} \equiv \left\{ \begin{smallmatrix} c \\ ab \end{smallmatrix} \right\} = \frac{1}{2} g^{cd} (\partial_b g_{ad} + \partial_a g_{db} - \partial_d g_{ab}). \quad (2.5)$$

As the Einstein–Hilbert Lagrangian density depends *linearly* on the second-order derivatives of the metric, one could discard these higher derivatives through a total divergence, the variation of which would not affect the equations of motion. Hence, one could start with the so-called ‘gamma-gamma’ first-order form of the Lagrangian density for gravity, which is given explicitly by

$$\mathfrak{L} = \sqrt{-g} g^{ab} \left(\Gamma^c_{ad} \Gamma^d_{bc} - \Gamma^c_{dc} \Gamma^d_{ab} \right). \quad (2.6)$$

This possibility elucidates why Einstein’s field equations are second-order instead of fourth-order differential equations. However, one should bear in mind that the ‘gamma-gamma’ Lagrangian density is no longer a scalar density.

Nevertheless, one aims at deriving Einstein’s equations in vacuum by requiring that the action (2.4) be stationary under arbitrary variations of the metric that vanish on the boundary. This is achieved with the help of the formula $\delta\sqrt{-g} = -\frac{1}{2}\sqrt{-g} g_{ab} \delta g^{ab}$ and the *Palatini equation*

$$\delta R^a_{bcd} = \nabla_c (\delta \Gamma^a_{bd}) - \nabla_d (\delta \Gamma^a_{bc}), \quad (2.7)$$

which can be easily derived in a locally geodesic coordinate system (see, e.g., [d’I92]) and the contraction of which is

$$\delta R_{ab} = \nabla_c (\delta \Gamma^c_{ab}) - \nabla_b (\delta \Gamma^c_{ac}). \quad (2.8)$$

The Hilbert metric variation of the action (2.4) is first written as¹²

$$\delta S = \int_{\mathcal{U}} d^4\Omega \left(\delta \mathfrak{g}^{ab} R_{ab} + \mathfrak{g}^{ab} \delta R_{ab} \right),$$

Making use of equation (2.8) and owing to the compatibility condition (in the form $\nabla_c \mathfrak{g}^{ab} = 0$) one can transform the second term of the integrand as a pure divergence; by Gauss’s theorem the corresponding integral becomes a surface integral over the boundary $\partial \mathcal{U}$ and vanishes because the variations are assumed to vanish on the boundary.¹³ Hence the variation of the Einstein–Hilbert action reduces to

$$\delta S = \int_{\mathcal{U}} d^4\Omega \mathfrak{G}_{ab} \delta g^{ab} \equiv 0,$$

¹²We recall that ‘Gothicised’ quantities denote tensor densities; for instance, $\mathfrak{A}^{ab} := \sqrt{-g} A^{ab}$, for an arbitrary tensor field A^{ab} .

¹³In fact, for general variations such that only the metric be held fixed on the boundary, this surface integral does not vanish; cf. our subsequent discussion on page 94 on the rôle of boundary terms.

where \mathfrak{G}_{ab} denotes the Einstein tensor density associated with the Einstein tensor

$$G_{ab} := R_{ab} - \frac{1}{2}Rg_{ab}.$$

Since the variations δg^{ab} and the region of integration \mathcal{U} are arbitrary, one concludes that the variational principle for the action (2.4) implies Einstein's vacuum field equations.

In keeping with the above variational principle, when matter comes into play, one must add to the gravitational Lagrangian density (2.1) an appropriate Lagrangian density \mathfrak{L}_M for the corresponding fields, which assumes a form that is a 'generalisation' of its special relativistic form—which depends primarily on the field variables, collectively called ψ —, achieved via the strong principle of equivalence according to the 'minimal coupling' rule:¹⁴

$$\eta_{ab} \longrightarrow g_{ab}, \qquad \partial_a \longrightarrow \nabla_a.$$

Observe that the order of the two steps is irrelevant as long as the connection is the Levi-Civita connection: For arbitrary connections the operation of lowering and raising indices does no longer commute with the operation of covariant differentiation. The total action is defined as $\int(\mathfrak{L} + \mathfrak{L}_M)$ and variation of the second term with respect to the metric defines the stress-energy tensor T_{ab} (cf. [LL89, §95]) so that the full field equations are $G_{ab} = T_{ab}$ supplemented by the equations of motion for the fields ψ . Furthermore, the generalised Bianchi identities (2.3) take the form of the contracted Bianchi identities, i.e. $\nabla^a G_{ab} = 0$, which in turn entail the covariant conservation of the stress-energy tensor, as a direct consequence of the invariance of the Einstein–Hilbert action under diffeomorphisms.

2.1.2 Einstein–Palatini variation

Consider a four-dimensional space-time manifold \mathcal{M} endowed with a Lorentzian metric g_{ab} but now assume that the connection ∇_c be an arbitrary *symmetric* connection, i.e. $\nabla_c g_{ab} \neq 0$ and zero torsion; hence $(\mathcal{M}, \mathbf{g}, \nabla)$ is an A_4 , i.e. an affine space provided with a symmetric linear connection (in which here a metric tensor is also defined), which is not necessarily a V_4 . In particular, no relationship is assumed *a priori* between the metric and the connection, i.e. they are independent from each other. The Einstein–Palatini, metric-affine variational principle proceeds with the specification of a Lagrangian density \mathfrak{L} that is constructed from the Riemann

¹⁴This prescription is not free from a certain ambiguity in the sense that there are other generalisations—e.g., conformal coupling—of the aforementioned special relativistic form that are indeed compatible with the basic postulate of general covariance.

tensor of the connection and also the metric; which is therefore assumed to be a functional of the metric, its covariant derivatives up to a certain order, the connection coefficients, and their derivatives up to a certain order, that is (formally)

$$\mathfrak{L} = \mathfrak{L}(\mathbf{g}, \nabla \mathbf{g}, \nabla \nabla \mathbf{g}, \dots; \Gamma, \partial \Gamma, \partial^2 \Gamma, \dots). \quad (2.9)$$

The analogue of the action functional (2.2) is

$$S[\mathbf{g}, \Gamma] = \int_{\mathcal{U}} d^4 \Omega \mathfrak{L}. \quad (2.10)$$

Its variation under arbitrary *independent* variations of the metric and the connection that vanish on the boundary $\partial \mathcal{U}$ is given by

$$\delta S[\mathbf{g}, \Gamma] = \int_{\mathcal{U}} d^4 \Omega \left(\mathfrak{A}_c^{ab} \delta \Gamma_{ab}^c + \mathfrak{B}_{ab} \delta g^{ab} \right),$$

where \mathfrak{A}_c^{ab} and \mathfrak{B}_{ab} are the Euler–Lagrange derivatives of \mathfrak{L} with respect to the connection and the metric respectively; hence the field equations are

$$\mathfrak{A}_c^{ab} = 0, \quad \mathfrak{B}_{ab} = 0,$$

sometimes called Γ - and \mathbf{g} -equations respectively.

As was first noted by Buchdahl, invoking such a method of variation in a gravitational theory is highly objectionable, for the Einstein–Palatini prescriptions ascribe to the variational principle the cumbersome task of picking out a specific class of spaces amongst all possible A_4 ’s [Buc60]: It is therefore implicitly assumed that one is dealing with a much broader geometrical setting than the familiar Riemannian space of general relativity; in fact, depending on the specific Einstein–Palatini Lagrangian, the general A_4 could degenerate into a more specialised space as for instance a Weyl space W_4 , or it could remain totally unspecified, with a completely arbitrary metric tensor. In our point of view such arbitrariness in the variational principle is obnoxious; we recommend that the specific geometry one is dealing with be fixed *ab initio* even though this is not the usual Riemannian geometry (cf. Subsection 2.2.3).

In the case of general relativity \mathfrak{L} can be chosen as the Hilbert–Palatini Lagrangian density $\mathfrak{L}_{\text{HP}} = \mathbf{g}^{ab} R_{ab}(\Gamma, \partial \Gamma)$, where the Ricci tensor depends on the connection coefficients and their first derivatives only; hence \mathfrak{L}_{HP} is regarded as a functional of the 10 metric components and the 40 connection coefficients. It turns out that the Einstein–Palatini method of variation is technically simpler than the Hilbert method of variation described in the previous subsection. Varying the Hilbert–Palatini action with respect to the metric g^{ab} one obtains directly

$$\delta S = \int_{\mathcal{U}} d^4 \Omega R_{ab} \delta \mathbf{g}^{ab} = \int_{\mathcal{U}} d^4 \Omega \mathfrak{G}_{ab} \delta g^{ab} \equiv 0, \quad (2.11)$$

whereas variation with respect to the affine connection Γ^c_{ab} yields, by virtue of the contracted Palatini equation (2.8),

$$\delta S = \int_{\mathcal{U}} d^4\Omega \mathfrak{g}^{ab} \delta R_{ab} = \int_{\mathcal{U}} d^4\Omega \mathfrak{g}^{ab} \left[\nabla_c (\delta \Gamma^c_{ab}) - \nabla_b (\delta \Gamma^c_{ac}) \right].$$

Integrating by parts and discarding the divergence term by the usual argument one obtains

$$\begin{aligned} \delta S &= \int_{\mathcal{U}} d^4\Omega \left[\nabla_b \mathfrak{g}^{ab} \delta \Gamma^c_{ac} - \nabla_c \mathfrak{g}^{ab} \delta \Gamma^c_{ab} \right] \\ &= \int_{\mathcal{U}} d^4\Omega \left(\delta^b_c \nabla_d \mathfrak{g}^{ad} - \nabla_c \mathfrak{g}^{ab} \right) \delta \Gamma^c_{ab} \equiv 0. \end{aligned}$$

Since the variations $\delta \Gamma^c_{ab}$, symmetric in a and b , and the region of integration \mathcal{U} are arbitrary, the symmetric part of the expression in round brackets must vanish, i.e.

$$\delta^b_c \nabla_d \mathfrak{g}^{ad} - \nabla_c \mathfrak{g}^{ab} = 0. \quad (2.12)$$

This latter equation is equivalent to the metricity condition $\nabla_c \mathfrak{g}^{ab} = 0 = \nabla_c g^{ab}$; hence the connection coefficients Γ^c_{ab} are necessarily the Christoffel symbols $\left\{ \begin{smallmatrix} c \\ ab \end{smallmatrix} \right\}$. Therefore one deduces that the field equations obtained from equation (2.11) coincide exactly with Einstein's vacuum field equations. This fact is the source of the commonly accepted belief that the Einstein–Palatini variational principle is equivalent to the Einstein–Hilbert variational principle. However, as we shall exemplify below, this is erroneous. As a matter of fact, for the Lagrangian $L = R$ in vacuum,¹⁵ the equivalence of the field equations turns out to be a mere coincidence. Still, in that very case the two variational methods are not equivalent because the corresponding boundary conditions are different. As mentioned above (cf. footnote (13)), in the purely metric situation the boundary term occurring in the process of variation does not vanish in general since the metric only is held fixed on the boundary. By contrast, in the metric-affine case the boundary term comes to naught since, in addition to the metric, the connection also is held fixed on the boundary. This means that one should have to add an *ad hoc* surface term in order to recover the Hamiltonian description of the fields at spatial infinity in the case of asymptotically flat space-times (cf. the discussion on boundary terms on page 94).¹⁶ On the other hand, inasmuch as quantum gravity is concerned, the

¹⁵Observe that the ‘gamma-gamma’ Lagrangian density is here ruled out as an alternative starting point for the derivation of Einstein's field equations because the difference between (2.6) and the Einstein–Hilbert Lagrangian density is a pure divergence only if the compatibility condition is assumed *ab initio* [ESU73].

¹⁶This undesirable feature is also present in the Ashtekar formalism, as a direct consequence of the use of a Hilbert–Palatini Lagrangian; see, e.g., [Bom88].

Einstein–Hilbert and Hilbert–Palatini Lagrangians—which are only equivalent ‘on shell’—will most probably give different theories since in the path-integral approach for instance one sums over all ‘off-shell’ contributions to the action. Furthermore, the choice of \mathfrak{L}_{HP} as the starting Lagrangian density for the Einstein–Palatini variational principle is very peculiar: The most general *second-order* (torsion-free) metric-affine Lagrangian density does in fact involve additional terms of the form $(\nabla \mathbf{g}) \cdot (\nabla \mathbf{g})$ (such as, e.g., $\nabla_a \sqrt{-g} \nabla_b g^{ab}$). In other words there are no selection rules that enable to pick out the Hilbert–Palatini Lagrangian density, by contrast to what happens in the metric case, where the requirement of having second-order field equations together with the covariance property uniquely determines the Einstein–Hilbert Lagrangian density (up to a cosmological constant). In an interesting paper Burton and Mann have recently found, for the aforementioned general second-order metric-affine Lagrangian density, the conditions under which the connection is in fact the Levi-Civita connection associated with the metric [BM98a]. They have shown that the compatibility condition, which arises naturally in the Hilbert–Palatini case, is in the more general situation a constraint that is induced by the breaking of a symmetry of the connection coefficients under the ‘deformation transformation’ $\Gamma_{ab}^c \longrightarrow \Gamma_{ab}^c + C_{ab}^c$ (where C_{ab}^c is an arbitrary tensor field symmetric in a and b). On the other hand, in the maximally symmetric case—i.e. when no constraints are imposed on the tensor field C_{ab}^c —the connection remains completely undetermined but can always be chosen so as to recover Einstein’s field equations.¹⁷

In the presence of matter fields there is an ambiguity in the prescription of the minimal coupling rule because the compatibility condition between the metric and the connection does not hold. Moreover, variation of the total action

$$S = \int_{\mathcal{U}} d^4\Omega \left[\mathfrak{R}(\mathbf{g}, \Gamma) + \mathfrak{L}_{\text{M}}(\mathbf{g}, \psi, \nabla \psi) \right], \quad (2.13)$$

gives the following pair of equations:

$$\mathfrak{G}_{ab} = \mathfrak{T}_{ab} := -2 \frac{\delta \mathfrak{L}_{\text{M}}}{\delta g^{ab}}, \quad (2.14a)$$

$$\delta_c^{(b} \nabla_d \mathfrak{g}^{a)d} - \nabla_c \mathfrak{g}^{ab} = \frac{\delta \mathfrak{L}_{\text{M}}}{\delta \Gamma_{ab}^c}, \quad (2.14b)$$

which are inconsistent in general owing to the fact that the purely geometric parts of these equations are projectively invariant whereas typical sources are not [HK78]. The equations (2.14) would be equivalent to the full Einstein field equations obtained via the Einstein–Hilbert variation only if the matter Lagrangian did not

¹⁷Curiously, the special choice $\Gamma_{ab}^c \equiv 0$ also turns the \mathbf{g} -equations into Einstein’s field equations.

depend explicitly on the connection, i.e. $\delta\mathfrak{L}_M/\delta\Gamma_{ab}^c \equiv 0$. In most circumstances this will be the case (e.g., scalar, Yang–Mills, electromagnetic fields) but one can pick out examples where this is not. For instance, when Einstein–Dirac fields are involved, the connection directly couples to the gravitational field thereby breaking the equivalence.¹⁸

Remark. In two dimensions in vacuum the Einstein–Palatini variation is unable to determine the connection completely [Des95]. This can be seen as follows. For any dimension n , the equation (2.12) implies that the connection coefficients are given by the formula

$$\Gamma_{ab}^c = \{^c_{ab}\} + \frac{1}{2}(\delta_a^c Q_b + \delta_b^c Q_a - g_{ab} Q^c), \quad (2.15)$$

where we have defined $Q_a := -\nabla_a(\ln \sqrt{-g}) = -\partial_a(\ln \sqrt{-g}) + \Gamma_a$ with $\Gamma_a := \Gamma_{ab}^b$. The trace of equation (2.15) is

$$\left(1 - \frac{n}{2}\right) [\partial_a(\ln \sqrt{-g}) - \Gamma_a] = 0$$

and identically vanishes when $n = 2$. Hence the Γ_a part of the connection is undetermined in two dimensions.

For completeness we reiterate that the Ashtekar formulation of canonical gravity is grounded on a generalised metric-affine variational principle, often referred to as Hilbert–Palatini variation [JS88, Pel94]. To be more specific, the basic independent (complex) fields are expressed in terms of soldering forms and self-dual connections instead of metrics and affine connections respectively [Ash86, Ash87]. (Those new canonical variables can be obtained by a succession of canonical transformations from the canonical variables of tetrad gravity [HNS89].) The Lagrangian for pure (complex) gravity is the so-called *self-dual Hilbert–Palatini Lagrangian* and the Ashtekar Hamiltonian is obtained upon an appropriate Legendre transformation.¹⁹ In Ashtekar’s formalism classical general relativity stems from the real sector of the complex theory. As a nonperturbative approach to canonical quantum gravity the Ashtekar Hamiltonian formulation does not involve generalised—e.g., higher-order—Lagrangians; therefore the only circumstances where the equivalence mentioned above breaks down arises when Dirac spinor fields are considered. In that case, because the spinors couple directly to the spin connection, the compatibility condition is altered by a term that gives torsion. Nevertheless, this problem can be avoided if an *ad hoc* term is added to the original Lagrangian [ART89].

¹⁸It can however be restored by ‘healing’ the action with *ad hoc* compensating terms [Wey50b].

¹⁹This formulation uses explicitly the aforementioned remarkable equivalence property of the Einstein–Hilbert and Einstein–Palatini variations.

2.2 Variational principles in higher-order gravity

2.2.1 Metric variation

In this subsection we write down the Euler–Lagrange derivatives stemming—via purely metric variation—from higher-order Lagrangians that are quadratic in the curvature tensors and from nonlinear gravitational Lagrangians.²⁰ Our main purpose is to provide the subsequent investigation of Chapter 4 with the explicit form of the field equations in vacuum and to enable a direct comparison with the equations that will be obtained in the next subsection via the metric-affine variational principle. In Subsection 2.2.3 we will show how the derivation of the fourth-order field equations can be overwhelmingly simplified by means the constrained first-order formalism.

In a four-dimensional Riemannian space-time $(\mathcal{M}, \mathbf{g})$ the general gravitational action that contains, besides the Einstein–Hilbert term $\mathfrak{L}_{\text{EH}} = \sqrt{-g} R$ (and possibly a cosmological constant) of general relativity, quadratic invariant combinations of the Riemann curvature tensor, Ricci tensor, and scalar curvature is

$$S = \int_{\mathcal{M}} d^4\Omega \left[\mathfrak{L}_{\text{EH}} + \gamma_1 \mathfrak{L}_1 + \gamma_2 \mathfrak{L}_2 + \gamma_3 \mathfrak{L}_3 \right], \quad (2.16)$$

where γ_i for $i = 1, \dots, 3$ are coupling constants and the quadratic Lagrangian densities are explicitly given by

$$\mathfrak{L}_1 := \sqrt{-g} R^2, \quad (2.17a)$$

$$\mathfrak{L}_2 := \sqrt{-g} R^{ab} R_{ab}, \quad (2.17b)$$

$$\mathfrak{L}_3 := \sqrt{-g} R^{abcd} R_{abcd}. \quad (2.17c)$$

(Note that a fourth possibility exists, namely $\mathfrak{L}_4 := \epsilon^{abcd} R_{ab}^{ef} R_{efcd}$, where ϵ^{abcd} is the Levi-Civita tensor, but it is of no interest according to parity conservation.)

The Lanczos action, which is constructed from the Gauss–Bonnet quadratic combination $R^{abcd} R_{abcd} - 4R^{ab} R_{ab} + R^2$, becomes a topological invariant in four dimensions: the Euler–Poincaré characteristic of the manifold (Gauss–Bonnet theorem). The corresponding Euler–Lagrange derivative is the Bach–Lanczos identity [Bac21, Lan38]:

$$\mathfrak{L}_{\text{BL}}^{ab} = \sqrt{-g} \left[C^{acde} C_{cde}^b - \frac{1}{4} g^{ab} C_{cdef} C^{cdef} \right]. \quad (2.18)$$

Owing to this remarkable property, only two of the quadratic invariants \mathfrak{L}_i are independent in four dimensions.

²⁰For a very detailed derivation of these results in the case of quadratic Lagrangians, we refer to Simon’s undergraduate thesis [Sim88].

Another interesting quadratic invariant is that constructed from the Weyl tensor, namely

$$\mathfrak{L}_c = \sqrt{-g} C_{abcd} C^{abcd}. \quad (2.19)$$

The associated action is the conformally invariant action in four dimensions, which is uniquely determined upon gauging conformal symmetry, i.e. upon promoting the global conformal group to a local gauge symmetry [KTN77, Rie86].

The fourth-order Euler–Lagrange derivatives corresponding to (2.17) are respectively:²¹

$$\mathfrak{L}_1^{ab} = \sqrt{-g} \left[\frac{1}{2} g^{ab} R^2 - 2R R^{ab} + 2\nabla^a \nabla^b R - 2g^{ab} \square R \right], \quad (2.20a)$$

$$\mathfrak{L}_2^{ab} = \sqrt{-g} \left[\frac{1}{2} g^{ab} R_{cd} R^{cd} - 2R^{bcad} R_{cd} + \nabla^a \nabla^b R - \square R^{ab} - \frac{1}{2} g^{ab} \square R \right], \quad (2.20b)$$

$$\begin{aligned} \mathfrak{L}_3^{ab} = \sqrt{-g} \left[\frac{1}{2} g^{ab} R^{cdef} R_{cdef} - 2R^{cdeb} R_{cde}{}^a - 4\square R^{ab} + 2\nabla^a \nabla^b R \right. \\ \left. - 4R^{bcad} R_{cd} + 4R^{ca} R^b{}_c \right], \end{aligned} \quad (2.20c)$$

where the box \square is the d'Alembertian second-order differential operator. The Euler–Lagrange derivative stemming from (2.19) is the tensor density associated with the Bach tensor B_{ab} [Bac21], which is defined by

$$\begin{aligned} B_{ab} &= 2\nabla^c \nabla^d C_{cabd} + C_{cabd} R^{cd} \\ &= -\square \left(R_{ab} - \frac{R}{6} g_{ab} \right) + \frac{1}{3} \nabla_a \nabla_b R + (C_{cabd} + R_{cabd} + R_{cbad}) R^{cd} \end{aligned} \quad (2.21)$$

and is symmetric, trace-free, and conformally invariant of weight -1 .

Aside from the quadratic invariants above, we also consider a nonlinear Lagrangian density that is a smooth arbitrary function of the scalar curvature, namely

$$\mathfrak{L} = \sqrt{-g} f(R), \quad \text{with } f'' \neq 0, \quad (2.22)$$

where a prime denotes differentiation with respect to the scalar curvature. The corresponding Euler–Lagrange derivative is

$$f' R_{ab} - \frac{1}{2} f g_{ab} - \nabla_a \nabla_b f' + g_{ab} \square f' = 0 \quad (2.23)$$

and was first obtained by Buchdahl [Buc70].

²¹This can be checked with the MATH-TENSOR package for MATHEMATICA; see, e.g., [TPH96] for the conformally invariant case.

2.2.2 Metric-affine variation

As already mentioned in the introduction of this chapter, such alternative variational principles as the purely affine or the metric-affine methods of variation were put forth in the early years of the relativistic gravitational theory. They were first analysed in the framework of quadratic gravitational Lagrangians by Weyl [Wey50a] and Eddington [Edd23]. Later, with the aim of obtaining second-order field equations different from Einstein's, Stephenson [Ste58, Ste59] and Higgs [Hig59] applied the Einstein–Palatini variational principle to the quadratic Lagrangians densities (2.17) and Yang investigated a theory based on the Lagrangian density (2.17c), by analogy with the Yang–Mills Lagrangian [Yan74]. However, as Buchdahl pointed out [Buc60], there was an error in Stephenson's method of variation—present in Yang's as well—as he imposed the metricity condition, i.e. the Levi-Civita connection, *after* the metric-affine variation. Buchdahl subsequently gave the correct field equations and demonstrated by means of specific examples that the Einstein–Palatini variational principle is not reliable in general [Buc79].²²

Recent investigations on those field equations derived from higher-order gravitational Lagrangians via the Einstein–Palatini variational principle may be reviewed briefly. The nonlinear $f(R)$ case has been studied by several authors. In a series of papers Shahid-Saless analysed the theory based on a $R + \gamma_1 R^2$ Lagrangian with matter [Sha87, Sha90, Sha91]. This was generalised to the $f(R)$ case by Hamity and Barraco who also studied the conservation laws and weak field limit of the resulting equations [HB93]. Ferraris, Francaviglia, and Volovich have recently shown that the Einstein–Palatini first-order formalism applied to general nonlinear $f(R)$ Lagrangians leads to a series of Einstein spaces, the cosmological constants of which being determined by the specific form of the function f [FFV94]. Similar results have been obtained in the case of $f(R_{ab}R^{ab})$ Lagrangians by Borowiec et al. [BFFV98, BF98]. First-order variations of a generic set of higher-order curvature terms appearing in string effective actions have been studied within the context of the cosmological constant problem by Davis [Dav98]. Tapia and Ujevic somehow extend the investigation made by Ferraris et al. on the universality property of Einstein spaces in the metric-affine setting [TU98]. As we shall see in Subsection 2.3.2, their claim that “it is also possible to incorporate a Weyl vector field” and “therefore the presence of an anisotropy” proves to be wrong in the light of the constrained metric-affine method in Weyl geometry.

In this subsection we first give the field equations that are derived from the quadratic Lagrangian densities (2.17) via the Einstein–Palatini variational principle

²²In that respect it is strange that none of the most recent works using the Einstein–Palatini method refers to Buchdahl's article.

[Buc79]. Next we analyse in greater detail the Einstein–Palatini variation of the nonlinear Lagrangian density (2.22). We also indicate how Buchdahl’s work can be extended to nonlinear Lagrangians of the type $f(R_{ab}P^{ab})$ [Mir97]; in particular, our analysis sheds another light on the ‘universality property’ most recently advocated by Ferraris et al. [FFV94, BFFV98] and by Tapia and Ujevic [TU98]. This impels us to present the Lagrange-multiplier version of the Einstein–Palatini method, namely the constrained first-order formalism (in Subsection 2.2.3), the consequences of which will be drawn in Section 2.3.

Quadratic case

Applying the Einstein–Palatini method of variation to the quadratic Lagrangian densities (2.17) one obtains the following sets of equations:²³

$$\delta\mathfrak{L}_1 \longrightarrow R\left(R_{(ab)} - \frac{1}{4}Rg_{ab}\right) = 0, \quad (2.24a)$$

$$\nabla_c(R\mathfrak{g}^{ab}) = 0; \quad (2.24b)$$

$$\delta\mathfrak{L}_2 \longrightarrow R_a{}^c R_{bc} + R_a{}^c R_{cb} - \frac{1}{2}R_{cd}R^{cd}g_{ab} = 0, \quad (2.24c)$$

$$\nabla_c\mathfrak{R}^{ab} = 0; \quad (2.24d)$$

$$\delta\mathfrak{L}_3 \longrightarrow 2R_{cda}{}^e R^{cd}{}_{be} - R_{acde}R_b{}^{cde} + R_a{}^c{}_{de}R_{cb}{}^{de} - \frac{1}{2}R_{cdef}R^{cdef}g_{ab} = 0, \quad (2.24e)$$

$$\nabla_d\mathfrak{R}_c{}^{(ab)d} = 0. \quad (2.24f)$$

For each Lagrangian density the second set of equations has been obtained after partial integration, use of the Palatini equation (2.7), and elimination of a trace. These equations have been first given by Stephenson [Ste58, Ste59] and Higgs [Hig59]. Their important features are threefold:

1. They are *conformally invariant*, that is invariant under conformal transformations $\tilde{g}_{ab} = \Omega^2(\mathbf{x})g_{ab}$, where $\Omega^2(\mathbf{x})$ is an arbitrary, strictly positive, scalar field. This can be easily understood on account of the fact that the affine connection is totally unrelated to the metric and because the Lagrangian densities from which they are derived are quadratic in the curvature. In a purely metric theory this property holds only for the Lagrangian density (2.19). Furthermore, Higgs was the first who showed that the solutions of equations (2.24) corresponding to R -squared and Ricci-squared Lagrangians are conformal to Einstein spaces with arbitrary cosmological constants [Hig59, Buc79].

²³Only the symmetric part of the Ricci tensor has been retained in \mathfrak{L}_2 ; cf. the remark on page 25.

2. They are second-order differential equations. This is due to the first-order nature of the Einstein–Palatini variation, which crumbles those double co-variant derivatives of the curvature tensors that typically occur in purely metric variations. In particular, they are obviously *not equivalent* to the fourth-order field equations (2.20) obtained via purely metric variations.
3. They do not yield the Levi-Civita connection as is the case for the linear Hilbert–Palatini Lagrangian and therefore their solutions are *not Riemann spaces*. However, in some specific cases it turns out that the underlined manifold is a ‘disguised’ W_4 , which can be brought onto an Einstein space upon a suitable conformal transformation (cf. the discussion on the nonlinear case below).

Remark. The Ricci tensor is not necessarily symmetric as in the Riemannian context; on writing $R_{(ab)} := P_{ab}$ and $R_{[ab]} := Q_{ab}$ we thereby see that to the Lagrangian density \mathfrak{L}_2 in V_4 there corresponds a whole family of Lagrangian densities in A_4 , namely $\mathfrak{L}_{2,\alpha} = \sqrt{-g} R_{ab}(P^{ab} + \alpha Q^{ab})$, where α is an arbitrary constant. In other words there are no selection rules that enable to choose $\alpha = 0$, i.e. \mathfrak{L}_2 , in the Einstein–Palatini variational principle. On the other hand, there are no a priori reasons whatsoever to discard other acceptable Lagrangian densities compatible with the Einstein–Palatini prescriptions. For example, one could start with that quadratic combination involving only the antisymmetric part of the Ricci tensor, namely

$$\mathfrak{L}_2^* := \sqrt{-g} R_{ab} Q^{ab}.$$

However, in that case the ensuing field equations impose only four conditions upon the forty Γ ’s and leave the metric tensor totally undetermined [Buc79]. This disconcerting situation also happens with the Ricci-squared Lagrangian: Equations (2.24c) and (2.24d) are fulfilled by any Ricci-flat, i.e. $R_{ab} = 0$, affine space A_4 whereas the metric tensor remains quite arbitrary. This sort of things never happens with purely metric variations, where the geometry is Riemannian from the outset. As Buchdahl, we claim that this degree of arbitrariness reflects discredit on the use of Einstein–Palatini variations in a theory of gravity.

Nonlinear case

Applying the Einstein–Palatini method of variation to the metric-affine analogue of the nonlinear Lagrangian density (2.22), that is

$$\mathfrak{L} = \sqrt{-g} f(g^{ab} R_{ab}(\Gamma)),$$

one obtains the following set of equations:

$$f' R_{(ab)} - \frac{1}{2} f g_{ab} = 0, \quad (2.25a)$$

$$\nabla_c (f' g^{ab}) = 0. \quad (2.25b)$$

Obviously, they differ from the Euler–Lagrange derivative (2.23). To see what these equations imply, we first expand equation (2.25b), viz.

$$f' \nabla_c g^{ab} + f'' g^{ab} \nabla_c R = 0.$$

Making use of the formulæ $\nabla_a \sqrt{-g} = \partial_a \sqrt{-g} - \sqrt{-g} \Gamma_a$ and $\nabla_a R = \partial_a R$ and assuming that $f' \neq 0$ we may write the latter equation as

$$\left[\partial_c (\ln \sqrt{-g}) + (\ln f')' \partial_c R - \Gamma_{cd}^d \right] g^{ab} + \partial_c g^{ab} + \Gamma_{cd}^a g^{db} + \Gamma_{cd}^b g^{ad} = 0. \quad (2.26)$$

Contracting with g_{ab} we see that Γ_c is a gradient:

$$\Gamma_c = \partial_c (\ln \sqrt{-g}) + 2 (\ln f')' \partial_c R.$$

This implies that the Ricci tensor is symmetric since $R_{[ab]} = \partial_{[a} \Gamma_{b]}$. Replacing Γ_c in equation (2.26) by the value given above and after little manipulation one obtains

$$\partial_c (f' g_{ab}) = f' (\Gamma_{ca}^d g_{db} + \Gamma_{cb}^d g_{ad}). \quad (2.27)$$

This suggests to define a conformally related metric with conformal factor f' ; indeed in that case the latter equation becomes

$$\partial_c \tilde{g}_{ab} = \Gamma_{ca}^d \tilde{g}_{db} + \Gamma_{cb}^d \tilde{g}_{ad}, \quad (2.28)$$

thereby implying that the covariant derivative of the new metric \tilde{g}_{ab} with respect to the connection ∇_c vanishes: hence the connection Γ_{ab}^c is the Levi-Civita connection of the metric \tilde{g}_{ab} . On the other hand, equation (2.26) is equivalent to

$$\nabla_c g^{ab} = \nabla_c (\ln f') g^{ab}, \quad (2.29)$$

which seems to show that the Einstein–Palatini variational principle has selected a W_4 , i.e. a Weyl space, with $Q_a = \nabla_a (\ln f')$ as the Weyl one-form. However, this is *not* a W_4 but a Riemann space with an ‘undetermined gauge’ [Sch54, p. 134]: Under a conformal transformation $\tilde{g}_{ab} = \Omega^2 g_{ab}$ in a W_4 the Weyl one-form transforms as $\tilde{Q}_a = Q_a - 2 \nabla_a (\ln \Omega)$; if Q_a is a *gradient*, it is always possible to choose the conformal factor in order to have $\tilde{Q}_a \equiv 0$, which amounts to consider a Riemann space—this is the case here since we can ‘gauge away’ the spurious Weyl one-form

by choosing precisely $\Omega^2 := f'$ as the conformal factor. On the other hand the analysis of the field equation (2.25a) is more straightforward. Taking its trace we find

$$f'(R)R = 2f(R). \quad (2.30)$$

This latter equation is identically satisfied (up to a constant rescaling factor) by the function $f(R) = R^2$, as is expected from the fact that any quadratic invariant metric-affine Lagrangian density is conformally invariant (cf. Point 1 on page 24). In that specific case the field equations (2.25a) reduce to

$$R_{ab} - \frac{1}{4}Rg_{ab} = 0, \quad (2.31)$$

provided that $f'(R) \neq 0$, and the conformal gauge degree of freedom is borne by the scalar curvature, which is assumed to be strictly positive. Hence, under an arbitrary conformal transformation $\tilde{g}_{ab} = k^2 Rg_{ab}$, with k^2 an arbitrary positive constant, the equation (2.31) becomes

$$\tilde{R}_{ab} - \frac{1}{4}\tilde{R}\tilde{g}_{ab} = 0, \quad (2.32)$$

where the conformal scalar curvature is constant, viz. $\tilde{R} \equiv k^{-2}$. Indeed, the equation (2.32) implies that the underlined manifold is an Einstein space with an arbitrary cosmological constant.

Remark. It is important to realise that, once the undetermined gauge has been removed, the conformal invariance is broken: The original ‘fake’ Weyl space has been replaced by an Einstein space—and Einstein spaces are of course not conformally invariant. In particular, the connection Γ_{ab}^c being the Levi-Civita connection associated with the conformal metric \tilde{g}_{ab} , it is totally inaccurate to perform an inverse ‘conformal transformation’ in which the connection remains frozen, as was the case in the departing counterfeit Weyl space. Strictly speaking it does not make any sense to go back to the original—illusory—space. In that respect what is found in the literature is either wrong (see e.g., Buchdahl’s conclusion after his relation (3.7) [Buc79]) or misleading (see e.g., Proposition 1 of Ferraris et al. [FFV94]).

If on the other hand one excludes the purely quadratic case and assume that the function $f(R)$ be given prior to the variation, then the trace equation (2.30) can be regarded as an algebraic equation to be solved for R . Denoting the resulting roots ρ_1, ρ_2, \dots one obtains a whole series of Einstein spaces, each characterised by a distinct constant scalar curvature. This situation was analysed by Ferraris et al. [FFV94] who extended Buchdahl’s investigation [Buc79]. However, if it happens for some root ρ_i to be such that $f'(\rho_i) = 0$, then the trace equation (2.30) entails

that $f(\rho_i) = 0$ as well. In that instance the field equations (2.25) leave both the metric and connection completely undetermined.²⁴

As a special case of the nonlinear theory, one can also apply the Einstein–Palatini variation to scalar-tensor Lagrangian densities. Consider for instance the Brans–Dicke action [BD61]:

$$S = \int d^4\Omega \sqrt{-g} \left(\phi^2 g^{ab} R_{ab} - 4\omega g^{ab} \nabla_a \phi \nabla_b \phi \right). \quad (2.33)$$

The appropriate conformal factor for which the connection Γ_{ab}^c is the Levi-Civita connection associated with the conformal metric \tilde{g}_{ab} turns out to be the Brans–Dicke scalar field. Rather than transforming the field equations one can first transform the Brans–Dicke action and thereafter perform the Einstein–Palatini variation. The resulting Lagrangian density is

$$\mathfrak{L}_{\text{BD}} = \sqrt{-g} \left(\tilde{R} - \frac{4\omega}{\phi^2} \tilde{g}^{ab} \partial_a \phi \partial_b \phi \right). \quad (2.34)$$

This corresponds to the ‘unit-transformed version’ of Brans–Dicke’s theory in which the gravitational constant is effectively constant and rest masses are varying (‘Einstein frame’) [Dic62].²⁵ As was first noticed by Van den Bergh, the peculiarity of the Brans–Dicke action is responsible for a curious fact: Although the purely metric variation and the Einstein–Palatini method are not equivalent when they are applied to the action (2.33), they yield the same dynamics if they are applied to the conformally transformed action constructed from (2.34); therefore the Einstein frame is singled out as the unit system in which both variational principles are equivalent [Ber81].²⁶

Generalisations of the nonlinear case

The above analysis can be performed on more general Lagrangian densities. By a completely analogous procedure one finds Einstein spaces for the following classes of Lagrangians:

- $L = f(R_{ab}P^{ab})$, where P_{ab} is the symmetric part of the Ricci tensor R_{ab} [BFFV98];

²⁴This situation is best illustrated with the Lagrangian $L = R^n$ for $n > 2$. Another interesting example is provided by the Lagrangian $L = aR^2 + bR + c$ with a , b , and c constant: Applying the Einstein–Palatini variation one obtains qualitatively different conclusions according to the specific values of the constants a , b , and c ; in particular, when $b^2 = 4ac$ there is only one condition, i.e. $R = \text{constant}$, and nothing else is determined.

²⁵The only difference lies in the coupling constant ω , which is equal to the *rescaled* Brans–Dicke coupling constant, i.e. $\omega \equiv \omega_{\text{BD}} - \frac{3}{2}$.

²⁶See also Burton and Mann’s recent investigation [BM98b].

- $L = f(\mathbf{R})$, where \mathbf{R} is any higher-order scalar constructed from the quantities $g^{ac}P_{cb}(\mathbf{\Gamma})$ [TU98];
- $L = f(R_{abcd}R^{abcd})$.

Firstly, we briefly consider the former case.²⁷ Let us define $r := R_{ab}P^{ab}$. Variation of the corresponding action yields the following \mathbf{g} - and $\mathbf{\Gamma}$ -equations:

$$f'P_{ac}P^c_b - \frac{1}{4}fg_{ab} = 0, \quad (2.35a)$$

$$\nabla_c(f'\mathfrak{P}^{ab}) = 0. \quad (2.35b)$$

From equation (2.35), after some manipulation, we conclude that Γ_a is a gradient; hence the Ricci tensor is symmetric and P_{ab} can be replaced by R_{ab} everywhere. Defining the ‘reciprocal’ tensor \hat{P}_{ab} (cf. [Buc79]) by $\hat{P}_{ac}P^{cb} = \delta_a^b$ and setting $p := \det P_{ab}$ we observe that the new metric that is defined by

$$\tilde{g}_{ab} := \frac{f'p^{1/2}}{\sqrt{-g}}\hat{P}_{ab} \quad (2.36)$$

or by

$$\tilde{g}^{ab} = \frac{\mathfrak{R}^{ab}}{f'p^{1/2}} \quad (2.37)$$

induces the connection Γ_{ab}^c as its associated Levi-Civita connection. Expressing the field equations (2.35a) in the conformal frame described by the metric \tilde{g}_{ab} we find anew an Einstein space, viz.

$$\tilde{R}_{ab} = \frac{1}{4} \frac{f\sqrt{-g}}{(f')^2 p^{1/2}} \tilde{g}_{ab}. \quad (2.38)$$

In the conformally invariant, i.e. quadratic ($f' \equiv 1$) case it is easy to show that the conformal factor can once again be chosen to remove the undetermined gauge that characterises the illusory Weyl space in the original frame. This conclusion also holds for the n -dimensional conformally invariant Lagrangians studied by Tapia and Ujevic [TU98].

For the latter instance in the list above, varying the corresponding action with respect to the metric and connection one obtains

$$-\frac{1}{2}fg_{ab} - f'R_a{}^{cde}R_{bcde} + f'R^c{}_{ade}R_{cb}{}^{de} + 2f'R^c{}_{dae}R_c{}^d{}_b{}^e = 0, \quad (2.39a)$$

$$\nabla_d(f'\mathfrak{R}_a{}^{(bc)d}) = 0, \quad (2.39b)$$

²⁷See Miritzis’s Ph.D. dissertation for a thorough investigation [Mir97].

but in contrast to the previous cases there exists no natural way to derive a conformal metric \tilde{g}_{ab} from the field equation (2.39b) unless the Weyl tensor vanishes [Dav98].

For completeness we mention that the inclusion of matter leads in general to inconsistencies. Moreover, in the nonlinear case the stress-energy tensor no longer satisfies the conservation equation; still, it is possible to define a new stress-energy tensor that is conserved but the physical interpretation of this generalised conservation law can be put in doubt since in the linearised theory for instance the ensuing equation of motion for test particles contains an additional term, which disagrees with Newton's law (see [HB93]). However, most recently, Borowiec and Francaviglia have shown that for those classes of nonlinear gravitational Lagrangians that give Einstein spaces it is also possible to derive the Komar expression for the energy-momentum complex [BF98].

In order to avoid the difficulties inherent to the Einstein–Palatini variational method, we now consider its Lagrange-multiplier version. This modification of the metric-affine variational principle enables one to choose from the outset the type of geometry one wants to deal with. As regards the path-integral approach to quantum gravity, for instance, this seems more consistent.

2.2.3 Constrained first-order formalism

As we have indicated in the previous subsections, when one applies the Einstein–Palatini variational principle one is often confronted with difficulties: Any departure from the Hilbert–Palatini Lagrangian density $\mathcal{L}_{\text{HP}} = \mathbf{g}^{ab} R_{ab}(\mathbf{\Gamma}, \partial\mathbf{\Gamma})$ brings forth cumbersome features. Nevertheless, the main shortcoming of the Einstein–Palatini method is not that the ensuing field equations are typically not equivalent to those that are derived from the ‘same’—in fact, they are different, since defined in different functional spaces—Lagrangian densities via the purely metric Einstein–Hilbert variational method but stems from the fact that it leads to certain indeterminacies, thereby vitiating its usefulness in a gravitational theory.

However that may be, our purpose is not to maintain the status quo; but, if one's aim is to examine generalisations of the orthodox variational principle, one ought to be careful and to proceed gradually, conveyed by the guiding principle that one should recover known results as special, limiting, cases of the extended framework. We shall prove in this subsection that one consistent way of performing this programme is that which proceeds with the Lagrange-multiplier version of the Einstein–Palatini variational principle, referred to hereafter as the *constrained first-order* method of variation [CMQ97].

The use of Lagrange multipliers in a variational principle is advocated when-

ever one wants to impose some constraint on the independent variables, for a straight enforcement is in general not consistent with the variation. In the context of gravity this was clearly stated for the first time—as far as we are aware—in Tonnelat’s book on Einstein’s attempts towards a unified theory of the ‘fundamental fields’ [Ton55]. In the context of Riemannian geometry this amounts to add to the Lagrangian density the compatibility condition as a constraint with Lagrange multiplier; next, one varies the resulting action with respect to the metric, connection, and Lagrange multiplier, considered as independent variables. When the constrained first-order method is applied to the Hilbert–Palatini Lagrangian, the Lagrange multiplier identically vanishes as a consequence of the field equations [Ray75]. This result strengthens the interpretation of the equivalence of the Einstein–Hilbert and Einstein–Palatini variations in vacuum general relativity as a pure coincidence. Applied to higher-order gravitational Lagrangians the constrained method proves to be technically much simpler than the purely metric equivalent variational method; this was demonstrated by Safko and Elston [SE76] and also by Ray [Ray78]. Nevertheless, the interesting applications of the constrained first-order method are those that are defined in the extended geometrical framework of MAG theories of gravity (see [HMMN95] and references therein).

Consider a four-dimensional space-time manifold \mathcal{M} endowed with a Lorentzian metric g_{ab} and its associated Levi-Civita connection, denoted hereafter $\overset{\circ}{\nabla}_c$ or, indifferently, $\{\overset{c}{ab}\}$.²⁸ Contradistinctively to the purely metric variation of Subsection 2.1.1 we want to relax the compatibility condition and allow for non-metricity during the variation; however, since we aim at recovering a specific type of space—e.g., Riemannian—after the variation, we must add to the original Lagrangian density \mathfrak{L} (now considered as a metric-affine functional of the metric, connection, and possibly matter fields ψ) the constraint

$$\mathfrak{L}_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) = \sqrt{-g} \Lambda_c^{ab} (\Gamma_{ab}^c - \{\overset{c}{ab}\} - C_{ab}^c), \quad (2.40)$$

where Λ_c^{ab} are Lagrange multipliers and C_{ab}^c is the difference tensor between the arbitrary symmetric connection Γ_{ab}^c and the Levi-Civita connection $\{\overset{c}{ab}\}$. For instance, in Riemannian geometry, i.e. $\overset{\circ}{\nabla}_c g_{ab} = 0$, (2.40) takes the form

$$L_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) = \Lambda_c^{ab} (\Gamma_{ab}^c - \{\overset{c}{ab}\}), \quad (2.41)$$

whereas in Weyl geometry, i.e. $\nabla_c g_{ab} = -Q_c g_{ab}$, it is

$$L_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) = \Lambda_c^{ab} \left[\Gamma_{ab}^c - \{\overset{c}{ab}\} - \frac{1}{2} g^{cd} (Q_b g_{ad} + Q_a g_{db} - Q_d g_{ab}) \right]. \quad (2.42)$$

²⁸The symbol ∇ henceforth refers to the independent connection that is varied in the constrained metric-affine variational principle.

The resulting metric-affine constrained action

$$S = \int_{\mathcal{M}} d^4\Omega \left[\mathfrak{L}(\mathbf{g}, \mathbf{\Gamma}, \psi) + \mathfrak{L}_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) \right], \quad (2.43)$$

must be varied with respect to the independent fields g^{ab} , Γ_{ab}^c , Λ_c^{ab} , and ψ . Variation with respect to the metric yields the \mathbf{g} -equations

$$\left. \frac{\delta \mathfrak{L}}{\delta g^{ab}} \right|_{\mathbf{\Gamma}} + \mathfrak{B}_{ab} = 0, \quad (2.44)$$

where the tensor density \mathfrak{B}_{ab} is defined by

$$\mathfrak{B}_{ab} = \sqrt{-g} B_{ab} := -\frac{1}{2} \sqrt{-g} \nabla^c (\Lambda_{bac} + \Lambda_{acb} - \Lambda_{cab}). \quad (2.45)$$

Variation with respect to the connection gives the $\mathbf{\Gamma}$ -equations

$$\left. \frac{\delta L}{\delta \Gamma_{ab}^c} \right|_{\mathbf{g}} + \Lambda_c^{ab} = 0. \quad (2.46)$$

Variation with respect to the matter fields ψ yields their respective equations of motion. Finally, variation with respect to the Lagrange multipliers restores the constraint (2.40).

Consider the specific case of Riemannian geometry.²⁹ Solving explicitly the $\mathbf{\Gamma}$ -equations (2.46) for the multipliers Λ_c^{ab} and substituting back the resulting expression into the \mathbf{g} -equations we should obtain field equations equivalent to those derived by ‘Hilbert varying’ the metric unconstrained action functional. This is expected by construction of the constrained variational method and can be checked explicitly on the previous higher-order Lagrangians densities. We first write down the resulting \mathbf{g} - and $\mathbf{\Gamma}$ -equations together with the actual values of the tensor B^{ab} for the Lagrangian densities (2.17):³⁰

$$\begin{aligned} \frac{1}{2} g^{ab} R^2 - 2R R^{ab} + B^{ab} &= 0, \\ \Lambda_c^{ab} &= (2g^{ab} \delta_c^d - g^{ad} \delta_c^b - g^{db} \delta_c^a) \nabla_d R, \\ B^{ab} &= -2g^{ab} \square R + 2\nabla^b \nabla^a R, \end{aligned} \quad (2.47a)$$

for the Lagrangian density \mathfrak{L}_1 ;

$$\begin{aligned} \frac{1}{2} g^{ab} R_{cd} R^{cd} - R^{ad} R_d^b - R^{bd} R_d^a + B^{ab} &= 0, \\ \Lambda_c^{ab} &= 2\nabla_c R^{ab} - \delta_c^a \nabla_d R^{db} - \delta_c^b \nabla_d R^{ad}, \\ B^{ab} &= -\square R^{ab} + 2\nabla_c \nabla^b R^{ac} - g^{ab} \nabla_d \nabla_c R^{cd}, \end{aligned} \quad (2.47b)$$

²⁹The generalisation to Weyl spaces will be considered in Subsection 2.3.2.

³⁰These formulæ correct Safko and Elston’s, which contain many misprints [SE76].

for the Lagrangian density \mathfrak{L}_2 ; and

$$\begin{aligned} \frac{1}{2}g^{ab}R_{cdef}R^{cdef} - 2R^{acde}R^b_{cde} + B^{ab} &= 0, \\ \Lambda_c^{ab} &= 2\nabla_d R_c^{abd} + 2\nabla_d R_c^{bad}, \\ B^{ab} &= 4\nabla_d \nabla_c R^{acbd}, \end{aligned} \quad (2.47c)$$

for the Lagrangian density \mathfrak{L}_3 . In the nonlinear case (2.22) we obtain likewise:

$$\begin{aligned} \frac{1}{2}fg^{ab} - f'R^{(ab)} + B^{ab} &= 0, \\ \Lambda_c^{ab} &= \frac{1}{2}(2g^{ab}\delta_c^d - g^{ad}\delta_c^b - g^{db}\delta_c^a)\nabla_d f', \\ B^{ab} &= -g^{ab}\square f' + \nabla^b \nabla^a f'. \end{aligned} \quad (2.48a)$$

It is straightforward to obtain the correspondence with the Euler–Lagrange derivatives (2.20) and (2.23) respectively by taking into account the Riemannian constraint and upon substituting in the \mathbf{g} -equations, within each set of (2.47) and (2.48), the respective expressions of B^{ab} . The outcome is:

$$\frac{1}{2}g^{ab}R^2 - 2RR^{ab} + 2\nabla^b \nabla^a R - 2g^{ab}\square R = 0, \quad (2.49a)$$

$$\frac{1}{2}g^{ab}R_{cd}R^{cd} - 2R^{bcad}R_{cd} + \nabla^b \nabla^a R - \square R^{ab} - \frac{1}{2}g^{ab}\square R = 0, \quad (2.49b)$$

$$\frac{1}{2}g^{ab}R_{cdef}R^{cdef} - 2R^{cdeb}R_{cde}^a + 4\nabla_d \nabla_c R^{acdb} = 0, \quad (2.49c)$$

$$f'R^{ab} - \frac{1}{2}fg^{ab} - \nabla^a \nabla^b f' + g^{ab}\square f' = 0. \quad (2.49d)$$

Strictly speaking, in comparison with the usual Hilbert variation, in all cases considered so far using the constrained first-order formalism, one starts from a *different* Lagrangian density, defined in a *different* functional space, follows a *different* variational method but nevertheless ends up in an *equivalent* set of field equations. Bearing this in mind, one can trace back this equivalence—which is not a mere formal coincidence—from the fact that all our Lagrangian densities are *diffeomorphism covariant*.

All previous cases can indeed be considered as specialisations of a very general Lagrangian n -form constructed locally as follows,

$$\mathbf{L} = \mathbf{L}(g_{ab}, \nabla_{a_1} g_{ab}, \dots, \nabla_{(a_1} \dots \nabla_{a_k)} g_{ab}, \psi, \nabla_{a_1} \psi, \dots, \nabla_{(a_1} \dots \nabla_{a_l)} \psi, \gamma). \quad (2.50)$$

More specifically, \mathbf{L} is a functional of the dynamical fields g_{ab} , ψ , finitely many of their covariant derivatives with respect to ∇_c , and also other ‘background fields’ collectively referred to as γ . Referring to ‘ g and ψ ’ as ‘ ϕ ’, L is called *f-covariant*, $f \in \text{Diff}(\mathcal{M})$, or simply diffeomorphism covariant if $\mathbf{L}(f^*(\phi)) = f^*\mathbf{L}(\phi)$,

where f^* denotes the induced action of the diffeomorphism f on the fields ϕ . (Note that this definition excludes the action of f^* on ∇ or the background fields γ .) It immediately follows that our previous Lagrangians satisfy the above definition and, as a result, are diffeomorphism covariant. It is a very interesting result, first shown by Iyer and Wald [IW94] that if \mathbf{L} as given in (2.50) is diffeomorphism covariant, then \mathbf{L} can be reexpressed in the form

$$\mathbf{L} = \mathbf{L}(g_{ab}, R_{bcde}, \overset{\circ}{\nabla}_{a_1} R_{bcde}, \dots, \overset{\circ}{\nabla}_{(a_1} \dots \overset{\circ}{\nabla}_{a_m)} R_{bcde}, \psi, \overset{\circ}{\nabla}_{a_1} \psi, \dots, \overset{\circ}{\nabla}_{(a_1} \dots \overset{\circ}{\nabla}_{a_l)} \psi), \quad (2.51)$$

where R_{abcd} is the Riemann curvature of $\overset{\circ}{\nabla}_c$ and $m = \max(k-2, l-2)$. Observe that everything is expressed in terms of the Levi-Civita connection of the metric tensor and also that all other fields γ are absent. Applying Iyer and Wald's theorem to our Lagrangians we immediately see that we could have reexpressed them from the outset in a form that involves only the Levi-Civita connection and not the original arbitrary connection ∇ , and vary them to obtain the corresponding 'Hilbert' equations. As we showed above, we arrived at this result by treating the associated Lagrangians as *different* according to whether or not they involved an arbitrary symmetric or a Levi-Civita connection.

Remark. This does not mean though that any metric-affine Lagrangian could be reexpressed as a purely metric Lagrangian. Here, we were allowed to apply Iyer and Wald's theorem because we started from a metric Lagrangian and *by construction* replaced it with a *constrained* metric-affine Lagrangian, where the connection is not in fact dynamical.

2.3 Conformal structure of nonlinear gravitational Lagrangians

2.3.1 Conformal equivalence properties

There is a huge literature involving conformal equivalence properties in the context of gravity theories.³¹ In this subsection we are mainly interested in recalling the well-known conformal equivalence property of nonlinear theories of gravity with Einstein's theory and additional scalar fields; in the next subsection we shall demonstrate how this classical result can be extended to Weyl geometry. We do not intend to discuss the 'physicality' issue arising from the aforementioned conformal equivalence, that is, the problem of determining which metric amongst the

³¹For a very recent and thorough review we refer the reader to the work of Faraoni, Gunzig, and Nardone [FGN98] and references therein.

equivalence class of conformally related metrics is the physical one. Since the early criticisms of Brans [Bra88], this question has raised a lot of controversies and misinterpretations. In the context of stringy gravity it seems to be a crucial—albeit often skirted—and fairly intricate issue (see however Dick’s constructive criticisms [Dic98]): One must indeed decide whether the rank-two tensor g_{ab} —which defines the ‘Jordan’, or ‘string frame’—occurring in the effective actions of string theory is to be interpreted as the physical metric tensor or rather as a unifying object conformally related to the genuine metric tensor \tilde{g}_{ab} of the space-time through additional scalar fields. In that respect most theoretical arguments seem to favour the (conformal) ‘Einstein frame’ as the relevant set of physical variables; this would also be true for a larger class of alternative theories of gravity including nonlinear theories of the $f(R)$ type, generalised scalar-tensor theories, and Kaluza–Klein theories after compactification of the extra dimensions: All these theories are dynamically equivalent—in the sense that their respective solution spaces are isomorphic to each other—to general relativity with scalar fields, which are still weird, hypothetical objects [Bra97].

The conformal equivalence of *vacuum* nonlinear gravity theories with general relativity plus a scalar field (see, e.g., [BC88]) can be proved within the extended framework of generalised scalar-tensor theories—which embody all theories involving scalar fields besides the metric—, described by the following generic Lagrangian [Hwa97]:

$$L = \frac{1}{2}f(\phi, R) - \frac{1}{2}\omega(\phi)g^{ab}\nabla_a\phi\nabla_b\phi - V(\phi). \quad (2.52)$$

The easiest way to proceed is to perform the appropriate conformal transformation on the Lagrangian itself, not on the field equations. Indeed, on defining the conformal factor as $\Omega^2 \equiv f' \equiv \exp(\sqrt{\frac{2}{3}}\psi)$ it is straightforward to obtain the conformally transformed Lagrangian corresponding to (2.52), namely

$$\tilde{L} = \frac{1}{2}\tilde{R} - \frac{1}{2}\frac{\omega}{f'}\tilde{g}^{ab}\tilde{\nabla}_a\phi\tilde{\nabla}_b\phi - \frac{1}{2}\tilde{g}^{ab}\tilde{\nabla}_a\psi\tilde{\nabla}_b\psi - \tilde{V}(\phi, \psi), \quad (2.53)$$

where the potential term is defined by

$$\tilde{V}(\phi, \psi) := \frac{1}{2(f')^2}(Rf' - f + 2V). \quad (2.54)$$

The original generalised Lagrangian (2.52) has thus been ‘cast’ into the Einstein–Hilbert Lagrangian with an additional scalar field ψ and an appropriate potential term $\tilde{V}(\phi, \psi)$. In most cases, introduction of a new scalar field $\tilde{\phi}$ reduces the expression (2.53) to the final form

$$\tilde{L} = \frac{1}{2}\tilde{R} - \frac{1}{2}\tilde{g}^{ab}\tilde{\nabla}_a\tilde{\phi}\tilde{\nabla}_b\tilde{\phi} - \tilde{V}(\tilde{\phi}), \quad (2.55)$$

provided that this new scalar field satisfies

$$d\tilde{\phi} = \sqrt{\frac{\omega}{f'}} d\phi^2 + d\psi^2.$$

As a special case of the generic situation above, the conformally transformed nonlinear $f(R)$ Lagrangian yields the field equations

$$\tilde{G}_{ab} = \nabla_a \phi \nabla_b \phi - \frac{1}{2} \tilde{g}_{ab} [(\nabla_c \phi \nabla^c \phi) - 2V(\phi)], \quad (2.56)$$

with potential

$$V(\phi) = \frac{1}{2} (f')^{-2} [R f'(R) - f(R)], \quad (2.57)$$

where it should be understood that R is superseded by ϕ through the inverse function to $f'(R)$.

The most important consequence of the conformal equivalence property in the context of higher-order gravity is that the original fourth-order field equations can be reduced to second-order equations, thereby simplifying the analysis of nonlinear gravity theories (see, e.g., [Cot90, Mir97] and references therein). On the other hand, the dynamical equivalence of nonlinear theories and general relativity plus additional scalar fields can be demonstrated by performing a Legendre transformation on the original set of variables (see, e.g., [Sok97] and references therein). This procedure—which amounts to transform the starting nonlinear theory into a scalar-tensor theory—was first used by Teyssandier and Tourrenc to solve the Cauchy problem for those theories [TT83] and is completely analogous to the generalised Ostrogradsky prescriptions studied in Chapter 3 (cf. p. 103); it can be generalised to Lagrangians that are functions not only of R but also $\square^k R$ for $k \in \mathbb{N}$ [Wan94]. Yet, it should be clear that the aforementioned Legendre transformation—sometimes referred to as a *Helmholtz formalism* [MS94]—does not play the rôle of the conformal transformation: Nonlinear gravity is *dynamically* equivalent to scalar-tensor gravity upon introducing additional scalar fields and the latter is then *conformally* equivalent to general relativity with one more scalar field [Wan94].³²

2.3.2 Generalised conformal structure in Weyl geometry

For the more general higher-order Lagrangians of the form $f(q)$ where $q = R$, $R_{ab}R^{ab}$, or $R_{abcd}R^{abcd}$ and where f is an arbitrary smooth function, the field

³²This slight difference is not merely conventional; it appears more clearly when one takes into account the boundary terms occurring in the respective actions.

equations obtained via the metric-connection formalism are of second order (cf. equations (2.39)) whereas the corresponding ones obtained via the usual metric variation are of fourth order. At first glance this result sounds very interesting since one could foresee that it would perhaps lead to an alternative way to ‘cast’ the field equations of these theories in a more tractable, reduced form than the one that is usually used for this purpose, namely the conformal equivalence theorem (cf. previous subsection). In this way, certain interpretational issues related to the question of the physicality of the two metrics associated with the conformal transformation would perhaps be avoided. Unfortunately, as indicated in Section 2.2, other difficulties arise when one uses the Einstein–Palatini method of variation, thereby vitiating its reliability as an alternative method to, for instance, reducing the complexity of the gravitational field equations. At the end of this subsection, we shall see that the origin of these troubles lies in the fact that the metric-affine variational principle is in fact a *degenerate* case of the constrained first-order formalism, therefrom unable to cope with more general geometrical settings such as ‘true’ Weyl spaces.

We are now interested in investigating the consequences of applying the constrained first-order formalism, defined in Subsection 2.2.3, to the case of Weyl geometry. We reiterate that a four-dimensional Weyl space W_4 is an affine space L_4 endowed with a linear symmetric and *semi-metric* connection, that is

$$\nabla_c g_{ab} = -Q_c g_{ab}, \quad (2.58)$$

where Q_c is the Weyl one-form that characterises the geometry. The Weyl constraint is (2.42); for convenience we recall its explicit form:

$$L_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) = \Lambda_c^{ab} \left[\Gamma_{ab}^c - \{^c_{ab}\} - \frac{1}{2} g^{cd} (Q_b g_{ad} + Q_a g_{db} - Q_d g_{ab}) \right]. \quad (2.59)$$

We apply the constrained first-order formalism to the nonlinear Lagrangian $L = f(R)$ in vacuum, making use of the contracted Palatini equation (2.8) and the following useful formulæ:

$$\begin{aligned} \delta_{\mathbf{g}} \{^c_{ab}\} &= \frac{1}{2} g^{cd} [\nabla_b (\delta g_{ad}) + \nabla_a (\delta g_{db}) - \nabla_d (\delta g_{ab})] \\ &\quad - \frac{1}{2} (Q_b g_{ad} + Q_a g_{db} - Q_d g_{ab}) \delta g^{cd}, \end{aligned} \quad (2.60a)$$

$$\begin{aligned} \delta_{\mathbf{g}} C_{ab}^c &= \frac{1}{2} (Q_b g_{ad} + Q_a g_{db} - Q_d g_{ab}) \delta g^{cd} \\ &\quad + \frac{1}{2} (Q_b \delta g_{ad} + Q_a \delta g_{db} - Q_d \delta g_{ab}) g^{cd}. \end{aligned} \quad (2.60b)$$

Variation of the nonlinear action

$$S = \int_{\mathcal{M}} d^4\Omega \left[\sqrt{-g} f(g^{ab} R_{ab}(\mathbf{\Gamma})) + \mathfrak{L}_c(\mathbf{g}, \mathbf{\Gamma}, \mathbf{\Lambda}) \right] \quad (2.61)$$

with respect to the Lagrange multipliers Λ_c^{ab} is trivial and recovers the definition of the Weyl connection in terms of the Levi-Civita connection and the Weyl one-form, that is

$$\Gamma_{ab}^c = \{^c_{ab}\} + \frac{1}{2}g^{cd}(Q_b g_{ad} + Q_a g_{db} - Q_d g_{ab}). \quad (2.62)$$

Taking into account that $\nabla_a \sqrt{-g} = -2Q_a \sqrt{-g}$, variation with respect to the metric g^{ab} yields the \mathbf{g} -equations

$$f' R_{(ab)} - \frac{1}{2}f g_{ab} + B_{ab} = 0, \quad (2.63)$$

where B_{ab} is defined by (2.45). Eventually, variation with respect to the connection brings forth the explicit form of the Lagrange multipliers, namely

$$\Lambda_c^{ab} = \delta_c^{(b}(Q^a)f' - \nabla^a)f' - g^{ab}(Q_c f' - \nabla_c f'). \quad (2.64)$$

Substituting back the latter result into equation (2.45) we find the expression of the tensor B_{ab} , that is

$$\begin{aligned} B_{ab} = & 2Q_{(a}\nabla_{b)}f' - \nabla_{(a}\nabla_{b)}f' + f'\nabla_{(a}Q_{b)} - f'Q_a Q_b \\ & - g_{ab}(2Q_c \nabla^c f' - Q^2 f' - \square f' + f'\nabla^c Q_c). \end{aligned} \quad (2.65)$$

Inserting this result into equation (2.63) we obtain the full field equations for the nonlinear Lagrangian $L = f(R)$ in the framework of Weyl geometry, viz.

$$f' R_{(ab)} - \frac{1}{2}f g_{ab} - \nabla_a \nabla_b f' + g_{ab} \square f' = M_{ab}, \quad (2.66)$$

where M_{ab} is defined by

$$\begin{aligned} M_{ab} := & -2Q_{(a}\nabla_{b)}f' - f'\nabla_{(a}Q_{b)} + f'Q_a Q_b \\ & + g_{ab}(2Q_c \nabla^c f' - Q^2 f' + f'\nabla^c Q_c). \end{aligned} \quad (2.67)$$

Note that the degenerate case of vanishing Weyl one-form coincides with the familiar field equations (2.23) obtained in the Riemannian framework.

As discussed in the previous subsection, those equations are conformally equivalent to Einstein's equations with a self-interacting scalar field as the matter source. We henceforth aim at generalising this important property in Weyl geometry. To this end, we define the metric \tilde{g}_{ab} conformally related to the metric g_{ab} with f' as the conformal factor. Owing to the fact that the Weyl one-form transforms as $\tilde{Q}_a = Q_a - \nabla_a(\ln f')$ and taking into account the formulæ $\tilde{\nabla}_a \equiv \nabla_a$, $\tilde{\square} \equiv \tilde{g}^{ab}\tilde{\nabla}_a \tilde{\nabla}_b = (f')^{-1}\square$, the field equations (2.66) become in the conformal frame

$$f' \tilde{R}_{(ab)} - \frac{1}{2} \frac{f}{f'} \tilde{g}_{ab} - \tilde{\nabla}_a \tilde{\nabla}_b f' + \tilde{g}_{ab} \tilde{\square} f' = \tilde{M}_{ab},$$

where the tensor \widetilde{M}_{ab} is given by

$$\begin{aligned}\widetilde{M}_{ab} = & f' \widetilde{Q}_a \widetilde{Q}_b - f' \widetilde{\nabla}_{(a} \widetilde{Q}_{b)} - \widetilde{\nabla}_a \widetilde{\nabla}_b f' \\ & + \widetilde{g}_{ab} (f' \widetilde{\nabla}^c \widetilde{Q}_c - f' \widetilde{Q}^2 + \widetilde{\square} f').\end{aligned}\quad (2.68)$$

Introducing the scalar field $\varphi := \ln f'$ and the potential $V(\varphi)$ in the ‘usual’ form, viz.

$$V(\varphi) = \frac{1}{2} (f')^{-2} [R f'(R) - f(R)], \quad (2.69)$$

we can rewrite the field equations in the final form

$$\widetilde{G}_{ab} = \widetilde{M}_{ab}(Q) - \widetilde{g}_{ab} V(\varphi), \quad (2.70)$$

where we have set

$$\widetilde{G}_{ab} = \widetilde{R}_{(ab)} - \frac{1}{2} \widetilde{R} \widetilde{g}_{ab} \quad (2.71a)$$

and

$$\widetilde{M}_{ab}(Q) = \widetilde{Q}_a \widetilde{Q}_b - \widetilde{\nabla}_{(a} \widetilde{Q}_{b)} + \widetilde{g}_{ab} (\widetilde{\nabla}^c \widetilde{Q}_c - \widetilde{Q}^2). \quad (2.71b)$$

Equivalently we could have obtained the field equations (2.70) from the corresponding conformally transformed action, via the constrained first-order formalism.

The field equations (2.70) are Einstein’s equations for a self-interacting scalar field matter source with a potential $V(\varphi)$ and a source term $\widetilde{M}_{ab}(Q)$ depending on the Weyl one-form \widetilde{Q}_a . If the geometry is Riemannian, i.e. $\widetilde{Q}_a = 0$, one recovers the standard conformal result. This will be the case only if the original Weyl one-form is a gradient, i.e. $Q_a \equiv \nabla_a \Phi$, since in that particular case it can be gauged away by the conformal transformation $\widetilde{g}_{ab} = (\exp \Phi) g_{ab}$ (cf. the discussion on page 26). This actually was the case of the Einstein–Palatini variational method applied to the Lagrangian $L = f(R)$, where the Weyl one-form turned out to be $Q_a = \nabla_a (\ln f')$. This fact shows unambiguously that *unconstrained* metric-affine variations of the Einstein–Palatini type cannot deal with a Weyl geometry and correspond to a degenerate case of the constrained first-order method: The field equations obtained from the former can be recovered within the constrained setting simply by choosing a very special form of the Weyl one-form [Que97] that makes the Weyl space degenerate in a Riemann space. As a direct consequence of our investigation, Tapia and Ujevic’s claim that, upon making use of the Einstein–Palatini variation, it is possible to incorporate a Weyl vector field—and therefrom account for the would-be observed anisotropy in the universe—is invalidated since

this vector field describes an undetermined gauge in a Riemann space and can therefore always be eliminated [QMC99].

Let us summarise the results obtained in this subsection. Our analysis has revealed that a consistent way to investigate generalised theories of gravity, without imposing *ab initio* that the geometry be Riemannian, is the constrained first-order formalism. Applications to quadratic and $f(R)$ Lagrangians in the framework of Riemannian and Weyl geometry show that the unconstrained Einstein–Palatini variational method is a degenerate case corresponding to a particular gauge and that the usual conformal structure can be recovered in the limit of vanishing Weyl one-form. (The generalisation of the result stated above to include arbitrary connections with torsion could be an interesting exercise.)

The physical interpretation of the source term in the field equations (2.66) is closely related to the choice of the Weyl vector field Q^a . However, it cannot be interpreted as a genuine stress-energy tensor in general since, for instance, choosing Q^a to be a unit timelike, hypersurface-orthogonal vector field, the sign of $M_{ab}Q^aQ^b$ depends on the respective signs of $f'(R)$ and ‘expansion’ $\nabla_a Q^a$.

The generalisation of the conformal equivalence theorem opens the way to analysing cosmology in the framework of these Weyl nonlinear theories by methods such as those used in the traditional Riemannian case (cf. [Cot97]). All the related problems could be tackled by leaving the conformal Weyl one-form \tilde{Q}_a undetermined, while setting it equal to zero will eventually lead to detailed comparisons with the results already known in the Riemannian case.

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Chapter 3

Hamiltonian formulation of higher-order theories of gravity

“And it is right that you should learn all things, both the persuasive, unshaken heart of Objective Truth, and the subjective beliefs of mortals, in which there is no true trust.”

— Parmenides of Elea, On Nature (Peri Physis).

WITHIN the realm of classical mechanics where it sprang up the Hamiltonian formalism chiefly served the purpose of a tool for tackling dynamical problems. So far Hamiltonian methods have demonstrated their ability to prove profound results—the renowned KAM theory, for example—and to solve otherwise intractable problems in various fields of mathematical physics: celestial mechanics, ergodic theory, statistical mechanics, and so forth [Arn76]. In addition the conceptual framework provided by the canonical formalism has become a convenient starting point for quantisation. This is the main reason why Hamiltonian methods have been applied to gravity as early as 1930 by Rosenfeld who constructed a quantum-mechanical Hamiltonian for the linearised theory of general relativity—though he did not make any attempt to develop a canonical version of the full theory. This last purpose was carried out with the pioneering works of Dirac, Bergmann and many others, and ended up as a consistent canonical formalism of Einstein’s general relativity: the celebrated ADM formalism. (For an historical perspective, see [DeW67].)

Besides the conceptual interest in the canonical version of general relativity, more restricted investigations using Hamiltonian methods as technical tools to tackle specific problems deserve consideration: Hamiltonian cosmology [Ugg97],

relativistic celestial mechanics and black hole physics (see references in [Bei94]), Hamilton–Jacobi theory in relativistic [Sal98] and string cosmology [Say97].

In this chapter we focus on the Hamiltonian formulation of theories with higher derivatives and its application to higher-order gravity theories. We do not address technical issues related to the quantisation of these theories; rather we concentrate on their classical structure, hoping to show that the canonical formulation can provide a very powerful method for reducing the order of the equations of motion. Applications of the Hamiltonian formalism to spatially homogeneous cosmologies is left to Chapter 4. We firstly review to some extent in Section 3.1 how to deal with first-order constrained Hamiltonian systems. Then in Section 3.2 we give a detailed analysis on the treatment of higher-order field theories by means of a generalisation of the so-called *Ostrogradsky construction*. Eventually we do attack the most important topic of this thesis in Section 3.3, namely the Hamiltonian formulation of higher-order theories of gravity. In particular, we exemplify the effectiveness of the Ostrogradsky method by building up a canonical version of gravity theories described by a Lagrangian that is an arbitrary function of the scalar curvature. This conveys us to prove the chief result of this chapter, that is the equivalence of the Ostrogradsky Hamiltonian formulation of general relativity and the well-known ADM canonical formalism [Que98].

3.1 Constrained Hamiltonian systems

3.1.1 Introduction

Physical theories of fundamental significance are invariant with respect to some group of *local* symmetry transformations—gauge transformations for Yang–Mills theories; space-time diffeomorphisms for gravity. Such theories are generically called *gauge theories* and can be thought of as theories in which the physical system under study is described by more variables than the number of physically independent degrees of freedom. The physically prevailing variables are those that are *gauge invariant* or, in other words, independent of the specific local symmetry transformation applied on the system. It is an essential characteristic of a gauge theory that the general solution to the equations of motion involves arbitrary functions of time: The local symmetry relates different solutions stemming from the same initial conditions. In the Lagrangian formalism this means that gauge theories are *singular systems* (cf. the remark on page 54).

It is unanimously acknowledged that the most exhaustive and reliable treatment of gauge systems is that which proceeds through the Hamiltonian formulation. Nevertheless it is worthwhile to start from the action principle in Lagrangian form

and proceed to the Hamiltonian formulation. Then the very presence of arbitrary time-dependent functions in the general solution of the equations of motion implies that the canonical variables are not all independent: There are conditions on the allowed initial momenta and positions. These relations amongst the canonical variables are called *constraints*. As a consequence, *all gauge theories are systems with constraints*—the converse, however, is not true. This is the reason why most textbooks on the quantisation of gauge systems proceed firstly to analysing Hamiltonian constrained systems—Henneaux and Teitelboim’s book is perhaps the best example in that respect [HT92]. (Historically, the classical Hamiltonian formalism has rather exclusively been considered as the fundamental setting on which canonical methods of quantisation are rooted.)

In contrast with the old approaches in theoretical physics, the aim of which was to reduce the number of variables entering in the play, the modern way of dealing with fundamental systems consists in introducing more powerful—gauge—symmetries while increasing the number of variables to make the description more transparent. This philosophy has culminated with the inception of the elegant and powerful BRST formalism; see, e.g., [HT92].

There exists a striking difference between gauge theories with *internal symmetries* and those which are *generally covariant*, that is, with reparameterisation invariance: In the former local symmetry transformations are generated by first-class constraints; in the latter the Hamiltonian itself is a constraint—the *super-Hamiltonian*. (In most circumstances, generally covariant systems do have a zero Hamiltonian; there exist, however, counterexamples to this property [HT92].) This raises the issue of interpreting time in generally covariant theories, for one is led to the question whether the Hamiltonian generates the dynamical time evolution or the kinematical local symmetries as the other first-class constraints usually do. In quantum gravity this issue is particularly puzzling since it is intrinsically linked to the various ways of foliating space-time in a one-parameter family of spacelike hypersurfaces; see, e.g., [AS91, Ish94], and references therein.

Circa 1950, the classical treatment of constrained systems was carried out by Dirac [Dir50, Dir58a, Dir64], Bergmann and collaborators [AB51, BG55]; almost instantaneously, Pirani and Schild applied Dirac’s methods to the gravitational field [PS50]. Dirac himself was mainly concerned in the Hamiltonian formulation of general relativity [Dir58b] and his leading efforts were completed in the sixties with the work of Arnowitt, Deser and Misner: the famous ADM formalism. Specifically they showed how to use the canonical setting to provide a rigorous characterisation of gravitational radiation and energy [ADM60, ADM62]. (As compared to the gravitational case, the application of Dirac’s methods to gauge theories—Maxwell electrodynamics and Yang–Mills theory—has not been so hastily initiated; see, e.g.,

[Sun82], and references therein.)

The geometrisation of the Dirac–Bergmann algorithm was achieved in the late seventies by Gotay, Nester, and Hinds [GNH78, GN79, GN80]. In the eighties, Batlle et al. obtained general proofs showing that the classical Hamiltonian and Lagrangian treatments of gauge theories are equivalent [BGPR86]. The Dirac–Bergmann theory opened the way up to the quantisation of constrained Hamiltonian systems even though canonical methods were hard to apply to theories of physical interest. Two distinct techniques emerged: the *Dirac method of quantisation*, in which the constraints are implemented as operators in Hilbert space, and the *reduced quantisation*, where the superfluous phase space degrees of freedom are eliminated before quantising, as is the case in the ADM approach. Their equivalence is still a matter of controversy; see references in García and Pons’s article [GP97]. The development of path-integral quantisation methods, incorporating the constraints in the definition of Feynman path integrals, and the extension of the formalism to include fermionic fields—upon the introduction of Grassmann variables—brought forth an appreciable advance which reached its apex with the advent of the powerful Hamiltonian BRST and Lagrangian *antifield* formalisms.

Besides the classical lectures of Dirac [Dir64] there are several excellent reviews on the treatment of constrained systems. Some focus more on systems with a finite number of degrees of freedom [SM74], others on field theories [HRT76], and some on both [Sun82, Gov91, HT92, Wip94, Bur97]. For generally covariant theories there exists a good monograph [GT90]. We draw on all these valuable sources to briefly summarise the theory of constrained systems, with the main purpose of defining the basic concepts and setting the notations that will be used throughout this chapter.

3.1.2 A short summary of Dirac–Bergmann theory

Action principle in Lagrangian form—Singular Lagrangians

Consider a conservative holonomic dynamical system the configuration of which at any instant of time is specified by K independent generalised coordinates q_k for $k = 1, \dots, K$; its time evolution can be derived from an action functional,

$$S[\gamma] = \int_{t_0}^{t_1} L(q_k(t), \dot{q}_k(t)) dt, \quad (3.1)$$

constructed from an appropriate Lagrange function $L(q, \dot{q})$ that depends explicitly on the generalised coordinates and their velocities;¹ it is understood that to any

¹At this stage we restrict the discussion to first-order Lagrangians with no explicit time dependence. Systems with higher derivatives are dealt with in Section 3.2. Moreover we assume

path $\gamma \equiv q_k(t)$ in configuration space that takes the initial and final values $q_k(t_0)$ and $q_k(t_1)$ one associates the value $S[\gamma]$ of the action, which is given by the integral (3.1). The classical motions of the system are those that make the action (3.1) stationary under variations $\delta q_k(t)$ of the generalised coordinates q_k that vanish at the endpoints t_0, t_1 . The necessary and sufficient conditions for the action (3.1) to be stationary are the Euler–Lagrange equations

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_k} \right) - \frac{\partial L}{\partial q_k} = 0 \quad \text{for } k = 1, \dots, K. \quad (3.2)$$

We can write equations (3.2) in more detail as

$$V_k(q, \dot{q}) - \sum_{l=1}^K W_{kl}(q, \dot{q}) \ddot{q}_l = 0 \quad \text{for } k = 1, \dots, K, \quad (3.3)$$

where we have introduced the quantities

$$V_k(q, \dot{q}) := \frac{\partial L}{\partial q_k} - \sum_{l=1}^K \frac{\partial^2 L}{\partial q_l \partial \dot{q}_k}, \quad (3.4a)$$

$$W_{kl}(q, \dot{q}) := \frac{\partial^2 L}{\partial \dot{q}_l \partial \dot{q}_k}. \quad (3.4b)$$

We immediately see from expressions (3.4) that all equations (3.3) are second-order, linearly independent equations, provided the Hessian matrix can be inverted, i.e. $\det W \neq 0$. Then the accelerations \ddot{q}_k at a given time are uniquely determined by the positions and the velocities at that time and the Lagrangian is said to be *regular*. The general solution to the equations of motion can thus be expressed in terms of $2K$ independent constants of integration which are fixed by the initial conditions. If, on the other hand, the determinant of the Hessian matrix is zero, the accelerations—and thus the dynamics—will not be uniquely determined by the positions and the velocities. The general solution to the equations of motion will then possibly involve arbitrary functions of time. In contradistinction with the former case the Lagrangian is said to be *singular*.

Henceforth we assume that the Lagrangian L is singular and that the rank of its associated Hessian matrix is constant everywhere on the velocity phase space and equal to $K - R$ for $R \in \mathbb{N}$, viz.

$$\text{rank} \left(\frac{\partial^2 L}{\partial \dot{q}_k \partial \dot{q}_l} \right) = K - R. \quad (3.5)$$

that there is a finite number of discrete degrees of freedom in order to render this summary as simple as possible.

Therefore, the matrix W has R null-eigenvectors $X^{(i)}$:

$$\sum_{l=1}^K X_l^{(i)}(q, \dot{q}) W_{kl}(q, \dot{q}) = 0 \quad \text{for } i = 1, \dots, R. \quad (3.6)$$

Contracting the Euler–Lagrange equations (3.3) with those eigenvectors we obtain necessary and sufficient conditions so that equations (3.3), interpreted as algebraic equations for the unknown \ddot{q}_k , have a solution; these are

$$\phi_i(q, \dot{q}) := \sum_{k=1}^K X_k^{(i)}(q, \dot{q}) V_k(q, \dot{q}) = 0 \quad \text{for } i = 1, \dots, R. \quad (3.7)$$

The independent conditions amongst equations (3.7) are called *Lagrangian constraints*.

Remark. Some null-eigenvectors can be determined from the generalised Bianchi identities, which are obtained through Noether’s second theorem; as a direct consequence, gauge theories are necessarily singular (see, e.g., [Wip94]).

Hamiltonian formalism

Primary constraints. The starting point for the Hamiltonian formalism is to define the canonical momenta by

$$p_k := \frac{\partial L}{\partial \dot{q}_k} \quad \text{for } k = 1, \dots, K. \quad (3.8)$$

We see that the vanishing of the determinant of the Hessian matrix W is precisely the condition that precludes the expression of the velocities as functions of the coordinates and momenta. In other words, the momenta (3.8) are not all independent in this case, and there exist amongst equations (3.8) some relations

$$\phi_i(q, p) = 0 \quad \text{for } i = 1, \dots, R, \quad (3.9)$$

which are assumed to be independent. The conditions (3.9) are called *primary constraints* to emphasise that the equations of motion were not used to obtain them. Through equations (3.9) these primary constraints define a $(2K - R)$ -dimensional submanifold—the *primary constraint surface*—, which we suppose to be smoothly embedded in phase space.

Generalised Legendre transformation—Canonical and Dirac Hamiltonians. The canonical Hamiltonian is introduced by

$$H_c := \sum_{k=1}^K \dot{q}_k p_k - L. \quad (3.10)$$

Even though H_c as defined by equation (3.10) is a function of the positions and the velocities, its dependence on (q, \dot{q}) is quite specific. Indeed, it is a remarkable property of the Legendre transformation that the velocities enter H_c only through the momenta given by definitions (3.8). This follows simply from the evaluation of the change δH_c induced by arbitrary independent variations of the positions and velocities. This means that H_c is a function of the p 's and q 's. However, it is not uniquely determined as a function of the phase space variables since the variations δp_k of the momenta are restricted to preserve the primary constraints (3.9). In other words, the canonical Hamiltonian is well defined only on the submanifold characterised by the primary constraints, and it can be extended arbitrarily off that manifold. The resulting function, which is not unique, is given by

$$H_{\mathcal{D}} := H_c + \sum_{i=1}^R \omega^i(q, p) \phi_i, \quad (3.11)$$

and is called a *Dirac Hamiltonian*. The canonical formalism remains unchanged under the replacement $H_c \rightarrow H_{\mathcal{D}}$.

The passage from $q, \dot{q}, L(q, \dot{q})$ to $q, p, H_{\mathcal{D}}(q, p)$ is called a *generalised Legendre transformation*. It enables to cast the action principle into Hamiltonian form: The Hamiltonian equations of motion

$$\begin{aligned} \dot{q}_k &= \frac{\partial H_c}{\partial p_k} + \sum_{i=1}^R \omega^i \frac{\partial \phi_i}{\partial p_k}, \\ \dot{p}_k &= -\frac{\partial H_c}{\partial q_k} - \sum_{i=1}^R \omega^i \frac{\partial \phi_i}{\partial q_k}, \end{aligned}$$

which are equivalent to the original Euler–Lagrange equations (3.2), can be derived from the variational principle

$$\delta \int_{t_0}^{t_1} \left(\sum_{k=1}^K \dot{q}_k p_k - H_c - \sum_{i=1}^R \omega^i \phi_i \right) dt = 0,$$

for arbitrary variations $\delta q_k, \delta p_k, \delta \omega^i$ subject only to the restriction that δq_k vanish at the endpoints. The variables ω^i , which render the Legendre transformation invertible, play here the rôle of Lagrange multipliers that are enforcing the primary constraints (3.9).

Poisson bracket—Weak and strong equations. Introducing the *Poisson bracket* of two arbitrary functions f, g , defined in phase space, by

$$\{f, g\} := \sum_{k=1}^K \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \sum_{k=1}^K \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k}, \quad (3.12)$$

we can formally write any equation of motion in the canonical formalism as

$$\dot{f} = \{f, H_{\mathcal{D}}\} = \{f, H_c\} + \sum_{i=1}^R \omega^i \{f, \phi_i\}. \quad (3.13)$$

At this stage it is useful to distinguish between *weak* and *strong* equations. The primary constraints (3.9) do not vanish identically throughout phase space and, in particular, they have nonzero Poisson brackets with the canonical variables. To take account of this property we write the primary constraints (3.9) as

$$\phi_i(q, p) \approx 0 \quad \text{for } i = 1, \dots, R, \quad (3.14)$$

where we have introduced the weak equality symbol “ \approx ”. More generally, two functions f, g that coincide on the primary constraint submanifold are said to be *weakly* equal, viz. $f \approx g$. On the other hand, an equation that holds throughout phase space is called *strong*, and the usual equality symbol “ $=$ ” is used in that case. Accordingly, we may write equations (3.11) and (3.13) respectively as

$$H_{\mathcal{D}} = H_c + \sum_{i=1}^R \omega^i(q, p) \phi_i \approx H_c, \quad (3.15a)$$

and

$$\dot{f} \approx \{f, H_{\mathcal{D}}\} \approx \{f, H_c\} + \sum_{i=1}^R \omega^i \{f, \phi_i\}. \quad (3.15b)$$

Dirac–Bergmann algorithm—Total Hamiltonian. A basic consistency requirement is that the primary constraints be preserved when time evolution is considered. This gives rise to the *consistency conditions* [Dir50, AB51]

$$\dot{\phi}_i \approx \{\phi_i, H_c\} + \sum_{j=1}^R \omega^j \{\phi_i, \phi_j\} \approx 0 \quad \text{for } i = 1, \dots, R, \quad (3.16)$$

which, for each value of the index i , correspond to one of the three possibilities:

1. Equation (3.16) is trivially satisfied, i.e. $0 \stackrel{!}{\approx} 0$.
2. Equation (3.16) is actually an equation to be satisfied by the Lagrange multipliers ω .
3. Equation (3.16) reduces to a relation independent of ω , that is, a new constraint on the p ’s and the q ’s which is said to be *secondary*—in contrast with “primary”—to emphasise that the equations of motion were used to obtain it.

For any secondary constraint we must again impose a consistency condition similar to (3.16) and perform the above analysis. This process must be repeated until all consistency equations have been exhausted. The outcome of this algorithm then consists in:

1. a complete set of R primary and S secondary constraints,

$$\phi_m \approx 0 \quad \text{for } m = 1, \dots, R + S = M; \quad (3.17)$$

2. restrictions on the Lagrange multipliers ω ,

$$\{\phi_m, H_c\} + \sum_{i=1}^R \omega^i \{\phi_m, \phi_i\} \approx 0 \quad \text{for } m = 1, \dots, M. \quad (3.18)$$

Conditions (3.18) may be thought of as a set of M nonhomogeneous linear equations in the R unknowns ω^i . (Note that since $R \leq M$ some compatibility conditions—i.e. further secondary constraints—could arise to ensure consistency; they must be treated through the algorithm as well.) The general solution of equations (3.18) is of the form

$$\omega^i \approx \mu^i + \sum_{\alpha=1}^A \lambda^\alpha \nu_\alpha^i, \quad (3.19)$$

where μ^i is a special solution of equation (3.18) and ν_α^i is a complete set of A linearly independent solutions of the associated homogeneous system

$$\sum_{i=1}^R \nu_\alpha^i \{\phi_m, \phi_i\} \approx 0. \quad (3.20)$$

Since the coefficients λ^α are totally arbitrary, equation (3.19) means that the multipliers ω have been resolved into one arbitrary part and one part that is fixed by the consistency conditions (3.18); for more details, see [HT92].

As a direct consequence of this analysis we may write the equation of motion (3.15b) equivalently as

$$\dot{f} \approx \{f, H_T\}, \quad (3.21)$$

with the *total Hamiltonian*,

$$H_T = H'_D + \sum_{\alpha=1}^A \lambda^\alpha \phi_\alpha, \quad (3.22)$$

which is defined as a sum of a Dirac Hamiltonian $H'_{\mathcal{D}}$,

$$H'_{\mathcal{D}} = H_c + \sum_{i=1}^R \mu^i \phi_i, \quad (3.23a)$$

and a specific linear combination of the primary constraints ϕ_α ,

$$\phi_\alpha = \sum_{i=1}^R \nu_\alpha^i \phi_i. \quad (3.23b)$$

Therefore the general solution to the canonical equations (3.21) will involve A arbitrary functions of time, as expected for a singular system.

First-class and second-class constraints. The concept of first-class and second-class functions on phase space was introduced by Dirac [Dir50, Dir64]; it plays a central rôle in the Hamiltonian formalism.

A function $f(q, p)$ is said to be *first class* if its Poisson brackets with every constraint vanish weakly, that is

$$\{f, \phi_m\} \approx 0, \quad \forall m = 1, \dots, R. \quad (3.24)$$

The set of first-class functions is closed under the Poisson bracket [Dir58a]. Directly available examples of first-class functions are $H'_{\mathcal{D}}$ and ϕ_α , defined by (3.23a) and (3.23b) respectively. Hence the total Hamiltonian (3.22) is the sum of the first-class Dirac Hamiltonian $H'_{\mathcal{D}}$ and an arbitrary linear combination of the primary first-class constraints ϕ_α . The number of arbitrary functions λ^α is thus equal to the number of primary first-class constraints. What makes first-class constraints so important is that they generate gauge transformations.² It indicates there is more than one set of canonical variables that corresponds to a given physical state. To overcome this ambiguity further restrictions may be imposed on the canonical variables: one proceeds to a *gauge-fixing* procedure (see, e.g., [Bur97]), which is not unique; its specific implementations actually determine the corresponding methods of canonical quantisation—e.g., Dirac quantisation, BRST method, reduced phase space quantisation [Bur82].³

Conversely, if there exists at least one constraint such that its Poisson bracket with f does not vanish weakly, then f is said to be *second class*. If χ_β denotes a

²For a more thorough discussion on the exact meaning of first-class constraints, especially with regard to some controversy found in the literature on the so-called Dirac's conjecture, see [Gov91, HT92].

³In the BRST approach, the phase space is extended rather than reduced.

complete set of second-class constraints, then the matrix C , the elements of which are precisely the Poisson brackets between the χ 's,

$$C_{\beta\beta'} = \{\chi_\beta, \chi_{\beta'}\}, \quad (3.25)$$

is nonsingular and its inverse is denoted as $C_{\beta\beta'}^{-1} \equiv C^{\beta\beta'}$. (This property may also serve as an alternative definition of the second-class constraints [Bur97].)

Dirac bracket. Second-class constraints are associated with redundant degrees of freedom which could be solved in terms of the other degrees of freedom provided that a generalised Poisson bracket referring to the remaining degrees of freedom only would be defined. This is achieved with the *Dirac bracket*, which is defined by

$$\{f, g\}_{\mathcal{D}} := \{f, g\} - \sum_{\beta, \beta'} \{f, \chi_\beta\} C^{\beta\beta'} \{\chi_{\beta'}, g\}, \quad (3.26)$$

for any arbitrary functions f, g on phase space, and which is always consistent with the second-class constraints.

Owing to definition (3.26), second-class constraints become strong equations, and we may write the equation of motion (3.21) as

$$\dot{f} \approx \{f, H^*\}_{\mathcal{D}}, \quad (3.27)$$

where H^* stands for any first-class Hamiltonian that generates time evolution: for instance, the total Hamiltonian H_T , or a more general choice with the *extended Hamiltonian* H_E which includes, in the linear combination of first-class constraints, *secondary* first-class constraints as well (see [HT92, Gov91] and footnote (2) on page 58).

Generally covariant systems

Systems that are invariant under arbitrary coordinate transformations are analogous to the parameterised form of mechanics in which the Hamiltonian and the time variable are introduced as a conjugate pair of canonical variables corresponding to a new degree of freedom. The resulting theory is invariant under an arbitrary reparameterisation. In field theory one can also introduce arbitrary labels for the spatial coordinates: The theory becomes invariant under an arbitrary change of the space-time coordinates, just like generally covariant theories. This is the reason why theories of gravity are said to be *already parameterised* systems. The 3 + 1-splitting of space-time, which is a crucial step towards their canonical formulation (see Section 3.3), has the virtue of “de-parameterising” the theory.

Time as canonical variable. Consider the action functional (3.1) and assume for simplicity that the Lagrangian L be regular. In order to raise the physical time t as a canonical variable we parameterise the theory with respect to a new time parameter τ such that $t = t(\tau)$ and $dt/d\tau \neq 0$. The original time is then interpreted as an additional generalised coordinate, i.e. $q_0 := t$. The action functional (3.1) thus becomes

$$S = \int_{\tau_0}^{\tau_1} d\tau q'_0 L(q_k, \frac{q'_k}{q'_0}) \equiv \int_{\tau_0}^{\tau_1} d\tau L_\tau(q_m, q'_m) \quad \text{for } m = 0, \dots, K, \quad (3.28)$$

where a prime denotes differentiation with respect to the parameter τ . It is invariant under any further reparameterisation $\tau^* = \tau^*(\tau)$. The conjugate momenta are given by

$$p_k^{(\tau)} = \frac{\partial L_\tau}{\partial q'_k} = \frac{\partial L}{\partial \dot{q}_k} = p_k \quad \text{for } k = 1, \dots, K, \quad (3.29a)$$

$$p_0^{(\tau)} = \frac{\partial L_\tau}{\partial q'_0} = L - \sum_{k=1}^K \frac{\partial L}{\partial \dot{q}_k} \dot{q}_k = -H(q_k, p_k). \quad (3.29b)$$

Hence relation (3.29b) is a primary constraint,

$$H_0(q, p) := p_0^{(\tau)} + H(q_k, p_k) \approx 0, \quad (3.30)$$

and the canonical Hamiltonian

$$H_c^{(\tau)} = \sum_{m=0}^K q'_m p_m^{(\tau)} - L_\tau = q'_0 H_0(q, p) \quad (3.31)$$

identically vanishes—a striking feature due to the parameterisation invariance. Since $H_0 \approx 0$ is the only constraint, the total Hamiltonian is simply

$$H_T^{(\tau)} = N(\tau) H_0(q, p), \quad (3.32)$$

where $N(\tau)$ is an arbitrary function which is interpreted as a Lagrange multiplier in the variational principle

$$\delta \int_{\tau_0}^{\tau_1} d\tau \left(\sum_{m=0}^K q'_m p_m^{(\tau)} - N(\tau) H_0(q, p) \right) = 0. \quad (3.33)$$

In particular, variation of (3.33) with respect to the momentum $p_0^{(\tau)}$ yields $N(\tau) = dt/d\tau$; hence the original canonical theory is recovered if we choose the synchronous temporal gauge, i.e. $N \equiv 1$.

Generalisation to field theory. The extension of the above parameterisation procedure to a field theory that is described by a Lagrangian density $\mathfrak{L}(\phi, \partial_\mu \phi)$ is achieved by interpreting the space-time coordinates as four new field variables, i.e. $x_\mu = x_\mu(\underline{x}_\nu)$. Thus there are four extra conjugate momenta; four constraint equations $H_\mu \approx 0$ are required to relate these momenta to the Hamiltonian density and the field momentum density. It is convenient to consider a foliation in terms of hypersurfaces which are labelled by constant ‘times’, that is $\underline{x}^0 = \text{const}$. Let n^α be the unit normal vector field to these hypersurfaces. Then we decompose the original set of constraints H_μ into their parts normal and tangential to the hypersurfaces, namely H_\perp and H_i for $i = 1, 2, 3$ respectively. The ensuing total Hamiltonian is

$$H_T = NH_\perp + \sum_{i=1}^3 N^i H_i. \quad (3.34)$$

In the context of general relativity the primary constraints H_\perp and H_i are called the *super-Hamiltonian* and the *super-momentum* respectively; see [MTW73, page 521]. The four corresponding Lagrange multipliers N^μ specify how to move forward in time from one hypersurface to the other as well as onto one and the same hypersurface—they are called the *lapse* and *shift* functions respectively; see, e.g., Kuchař’s review for a very detailed account [Kuc81].

3.2 Theories with higher derivatives

3.2.1 Introduction

The Hamiltonian formulation of theories with higher derivatives was firstly developed by Ostrogradsky almost one and a half century ago [Ost50]. Basically, the Ostrogradsky method [DNF82, Whi37] is adapted only to systems described by a *regular* Lagrangian, that is, a Lagrange function the associated Hessian matrix of which with respect to the highest-order time derivatives has a nonzero determinant. The underlying idea of this method—and of its subsequent generalisations—consists in introducing besides the original configuration variables a new set of coordinates that encompasses each of the successive time derivatives of the original Lagrangian coordinates so that the initial higher-order regular system be reduced to a first-order system. In order to recover the standard interpretation of the old coordinates when time evolution is considered it is essential to insert into the formalism the definition of the new coordinates in terms of the old ones by means of a Lagrange-multiplier technique. As a direct consequence, the auxiliary degrees of freedom that enable the order-lowering in the initial Lagrangian are constrained: One must resort to Dirac’s approach for building up a consistent Hamiltonian formalism [GR94].

It seems that the very first use of Ostrogradsky’s method was undertaken by Kerner in an attempt to develop a Hamiltonian formalism for Wheeler–Feynman electrodynamics (cited in [JLM86]). It is a remarkable result indeed in relativistic particle dynamics that, for conservatively interacting particles, there does not exist an ordinary single-time Lagrangian or Hamiltonian description if the position coordinates belong to a Lorentz frame. Rather, it turns out that in a local-in-time representation all higher time derivatives must appear in the Lagrangian, which is therefore an infinite-order Lagrange function. Now, because infinite-order Lagrangian systems exhibit cumbersome mathematical features, there have been many attempts to weed out all higher time derivatives occurring in the higher-order equations of motion by utilising the equations of motion of lower orders. In such a reduction process the question naturally arises whether the original infinite-order Lagrangian can also be reduced to an ordinary Lagrangian. The answer is not trivial for, in general, a system of second-order ordinary differential equations does not admit an ordinary Lagrangian description. On the contrary, the existence of a Hamiltonian formulation is warranted owing to the Lie–König theorem [Whi37]. Moreover, as Jaén et al. pointed out, a straight substitution into the equations of motion implies the intromission of some constraints that modify the very nature of the variational principle underlying the Lagrangian formalism. It is precisely for this reason that Jaén et al. tackled the problem of finding the reduced Hamiltonian by means of the techniques of constrained Hamiltonian dynamics together with the Ostrogradsky method in the case of Wheeler–Feynman electrodynamics [JLM86] (see also Ellis’s canonical formalism for a second-order Lagrangian [Ell75]).

More generally, in the problem of reduction of higher-order Lagrangians describing the dynamics of systems of point particles, which are given as formal power series in some ordering parameter, Damour and Schäfer developed a new method, called ‘the method of redefinition of position variables’, that enabled them to eliminate consistently the higher time derivatives, directly at the Lagrangian level [DS91].

This type of reduction process was also examined by Grosse-Knetter in the context of general effective higher-order Lagrangians [Gro93, Gro94]. However, it must be objected that Grosse-Knetter’s treatment is not reliable. The major criticism that one could raise has to do with the simplifying assumption that $\delta^4(0)$ -terms occurring in the path-integral formalism may be neglected *on the mere analogy* of what happens in the first-order case. As a matter of fact these terms should not be discarded unless a suitable regularisation method would be successfully applied. Beyond that particular point, the proofs—quite elusive, by the way—make an inappropriate use of the results obtained by Damour and Schäfer, which are valid only for effective Lagrangians that can be written as formal power series.

Furthermore no scrupulous constraint analysis is performed when discussing the equivalence of Lagrangian and Hamiltonian path-integral quantisations. In that respect the claim that any higher-order effective Lagrangian can be reduced to a first-order one *without* introducing extra degrees of freedom—by the way, “eliminating the unphysical effects associated with Ostrogradsky additional degrees of freedom” [Gro94]—is not proved by any rigorous analysis whatsoever.

On the other hand, Gitman et al. have worked out a consistent method of building up a Hamiltonian formalism for any constrained system with higher derivatives (see [GT90] and references therein). Buchbinder and Lyakhovich improved the treatment in a form that is more appropriate for theories of gravity (see [BOS92] and references therein); more specifically, they applied the method to the most general quadratic gravitational action in four dimensions [BL87]; then, with Karataeva, they extended the analysis to the realm of multidimensional quadratic gravity [BKL91]. Within the particular subclass of singular second-order Lagrangians Nesterenko [Nes89] and Batlle et al. [BGPR88] discussed, in a more geometrical setting, the relationship between the Lagrangian and Hamiltonian frameworks; Galvã and Lemos examined the peculiar case of singular second-order Lagrangians that differ from a regular first-order Lagrangian by a total time derivative of a function of both the coordinates and velocities [GL88]; prompted by the strange superstition that dealing with Ostrogradsky Lagrangian constraints ravel the mind, Schmidt contrived an ‘alternate Hamiltonian formalism’ [Sch97] (see also Kasper’s similar approach [Kas97]).

In the general case Pons achieved a rigorous unification of the Dirac formalism for constrained systems and the Ostrogradsky method for higher-order Lagrangians [Pon89]. Saito et al. developed a similar formalism that they applied to the aforementioned case of a Lagrangian describing the gravitational interaction of two point particles [SSOK89].

Subsequent formal investigations inspired by the Ostrogradsky method may be reviewed briefly. In order to study the interplay of higher-order Lagrangian and Hamiltonian formalisms, Gràcia et al. introduced ‘partial Legendre–Ostrogradsky transformations’ and constructed some interesting geometric structures [GPR91]; within this geometrisation scheme Gràcia and Pons extended previous significant results [GP92] to the study of Noether-symmetry transformations for higher-order Lagrangians [GP95]. Chitaya et al. have analysed the constrained Ostrogradsky method for constructing the generators of local symmetry transformations [CGS97]. Kaminaga has showed that the adjunction of total derivative terms to a higher-order Lagrangian does not affect either the classical or the quantum canonical structure of the system [Kam96].⁴ Nakamura and Hamamoto have analysed the

⁴In the Lagrangian formalism this problem is trivial: The equations of motion are not affected

path-integral formalisms associated with different variants of the Ostrogradsky construction: the standard, the constrained, and the generalised methods respectively [NH96]. Most recently, Nirov has elaborated a BRST formalism for systems that are invariant under gauge transformations with higher-order time derivatives of gauge parameters [Nir96, Nir97]; Pimentel and Teixeira have generalised the Hamilton–Jacobi approach for higher-order singular systems [PT98].

Very few applications of the Ostrogradsky method to specific higher-order field theories have been actually undertaken; for instance, de Urries and Julve have demonstrated the physical equivalence of relativistic scalar field theories with higher derivatives and their reduced second-order counterpart: They compare the standard Ostrogradsky procedure to a Lorentz-invariant method based on the use of the so-called ‘Helmholtz Lagrangian’ [dUJ98]. In the context of higher-order theories of gravity, especially in quantum cosmology, the situation is not very different. For a quadratic Lagrangian involving R and R^2 terms Kasper has compared Buchbinder and Lyakhovich’s generalised Ostrogradsky formalism to another method that is characterised by the introduction of a scalar field at the Lagrangian level; he obtains approximate solutions to the Wheeler–DeWitt equation, with a closed FLRW ansatz [Kas93] (Kasper’s analysis has been improved by Pimentel and Obregón who solved the same equation analytically [PO94]). Pimentel et al. have obtained solutions to the Wheeler–DeWitt equation corresponding to the Taub model in the case of a pure quadratic R^2 Lagrangian [POR97]. In a very recent work, Ezawa et al. have developed a canonical formalism for $f(R)$ theories of gravity [EKK⁺98]; the formulation presented in Section 3.3 is in total agreement with their approach although a slightly different choice for the canonical variables does actually simplify the analysis.⁵

Remark. The Ostrogradsky method has also been used to highlight the fundamental drawbacks inherent in higher-order theories [EW89, Sim90, Sch94, Sch97].

3.2.2 Ostrogradsky’s method for regular systems

Consider a system with a finite number K of discrete degrees of freedom represented by generalised coordinates x_k for $k = 1, \dots, K$ in configuration space; for the sake of clarity we assume that these coordinates are commuting variables though it should be clear that exactly the same considerations are valid for commuting and anticommuting degrees of freedom, as well as for infinite discrete or noncountable set of coordinates—the former case corresponds to the treatment of

by the addition of a total derivative term to the Lagrangian.

⁵The completion of this work was achieved during a visit at the Department of Mathematics of the University of the Aegean (Samos, Greece) in May 1996.

bosonic and fermionic types of degrees of freedom and the latter typically that of field theories. Consider now that the system under study be described by some time-independent—it is for convenience only that we restrict the analysis to time-independent Lagrangians; time-dependent Lagrange functions can also be treated along the same lines as developed hereafter—*regular* Lagrange function

$$L\left(x_k, \dot{x}_k, \ddot{x}_k, \dots, x_k^{(\alpha_k)}\right) \quad \text{for } \alpha_k \geq 1 \text{ and } k = 1, \dots, K, \quad (3.35)$$

where we adopt the convention $\left(\frac{d}{dt}\right)^i x_k = x_k^{(i)}$. The index α_k denotes the maximal order of all time derivatives of the coordinate x_k appearing explicitly in the Lagrangian (3.35). (Note that when $\alpha_k = 1$ for all degrees of freedom one recovers as a special case of the present general treatment the familiar situation encountered in classical mechanics for first-order Lagrangians.) In the original formulation of the Ostrogradsky method it is also assumed that the Lagrange function does depend on at least the first-order time derivative of each degree of freedom in order to prevent the occurrence of undesirable constraints.

As usual we assume that the dynamical time evolution of the system is obtained upon extremising the action functional constructed from the Lagrangian (3.35) under variations $\delta x_k(t)$ of the configuration variables x_k . The variational principle yields the $2N^{\text{th}}$ -order Euler–Lagrange equations

$$\sum_{\sigma_k=0}^{\alpha_k} (-1)^{\sigma_k} \left(\frac{d}{dt}\right)^{\sigma_k} \frac{\partial L}{\partial x_k^{(\sigma_k)}} = 0, \quad N = \sup_k \{\alpha_k\}. \quad (3.36)$$

Adopting Ostrogradsky’s prescriptions we introduce new quantities p_{k,γ_k} for $\gamma_k = 0, \dots, (\alpha_k - 1)$ (which depend on derivatives of the coordinates x_k up to order $2\alpha_k - \gamma_k - 1$) that are defined by the following recursion relations

$$p_{k,\alpha_k-1} = \frac{\partial L}{\partial x_k^{(\alpha_k)}}, \quad (3.37a)$$

$$p_{k,\beta_k-1} = \frac{\partial L}{\partial x_k^{(\beta_k)}} - \frac{d}{dt} p_{k,\beta_k} \quad \text{for } \beta_k = 1, \dots, (\alpha_k - 1). \quad (3.37b)$$

We can now prove the following result (see, e.g., [Whi37, pp. 265]).

Ostrogradsky’s theorem. *Let L be a regular Lagrangian depending on generalised coordinates x_k and their time derivatives up to order $\alpha_k \geq 1$ for $k = 1, \dots, K$. Consider new quantities p_{k,γ_k} for $\gamma_k = 0, \dots, (\alpha_k - 1)$ that are introduced by the recursion relations (3.37). The Euler–Lagrange equations (3.36) derived from L are equivalent to the system of canonical equations that is obtained from the Hamiltonian*

$$H = \sum_{k=1}^K \sum_{\gamma_k=0}^{\alpha_k-1} \dot{x}_k^{(\gamma_k)} p_{k,\gamma_k} - L.$$

Proof. Owing to the recursion relations (3.37) the Euler–Lagrange equations (3.36) take the simple form

$$\frac{\partial L}{\partial x_k} - \frac{d}{dt} p_{k,0} = 0 \quad \text{for } k = 1, \dots, \alpha_k, \quad (3.38)$$

which is reminiscent of Hamilton’s equations of motion. To make this statement more specific consider the quantity defined by

$$H = \sum_{k=1}^K \sum_{\gamma_k=0}^{\alpha_k-1} \dot{x}_k^{(\gamma_k)} p_{k,\gamma_k} - L, \quad (3.39)$$

where the variables p_{k,γ_k} are determined through the recursion relations (3.37). As it stands, the function H should depend explicitly on variables x_k and their derivatives up to order $(2\alpha_k - 1)$, on account of the definitions (3.37) for the quantities p_{k,γ_k} the dependence of which on the velocities $x_k^{(\sigma_k)}$ for $\sigma_k = 1, \dots, (2\alpha_k - 1)$ is manifest. However, taking the differential of the function H defined above we obtain the identity

$$dH = \sum_{k=1}^K \sum_{\gamma_k=0}^{\alpha_k-1} \left(x_k^{(\gamma_k+1)} dp_{k,\gamma_k} - \dot{p}_{k,\gamma_k} dx_k^{(\gamma_k)} \right) - \sum_{k=1}^K \left(\frac{\partial L}{\partial x_k} - \dot{p}_{k,0} \right) dx_k, \quad (3.40)$$

where the last sum turns out to be a combination of the Euler–Lagrange equations. This result establishes that the function H defined by (3.39) depends on variables $x_k^{(\sigma_k)}$ for $\sigma_k = 0, \dots, (2\alpha_k - 1)$ only through a dependence of the variables $x_k^{(\gamma_k)}$ and p_{k,γ_k} themselves, viz. $H = H(x_k^{(\gamma_k)}, p_{k,\gamma_k})$. Note that this property holds even in the case of a singular Lagrangian; however, here, unhampered by any degeneracies we are able to perform a suitable Legendre transformation: We regard variables $(x_k^{(\gamma_k)}, p_{k,\gamma_k})$ as being canonically conjugate pairs and we only solve for the first-order time derivatives of the variables $x_k^{(\alpha_k-1)}$ in terms of variables p_{k,α_k-1} and variables $x_k^{(\gamma_k)}$; throughout this procedure the latter variables must be considered as independent of one another rather than being time derivatives of order γ_k of the coordinates x_k . Finally the identity (3.40) shows that the Euler–Lagrange equations (3.36) are equivalent to the system of canonical equations

$$\dot{x}_k^{(\gamma_k)} = \frac{\partial H}{\partial p_{k,\gamma_k}}, \quad (3.41a)$$

$$\dot{p}_{k,\gamma_k} = -\frac{\partial H}{\partial x_k^{(\gamma_k)}}, \quad (3.41b)$$

obtained from the Hamiltonian (3.39). ■

Let us summarise the whole Ostrogradsky procedure. Firstly, we introduce the *conjugate momenta* p_{k,α_k-1} with definition (3.37a), where it should be understood that the variables $(x_k, \dot{x}_k, \dots, x_k^{(\alpha_k-1)})$ are independent. Owing to the fact that our Lagrangian is regular, we are able to invert relations (3.37a) for the velocities $\dot{x}_k^{(\alpha_k-1)}$, viz.

$$x_k^{(\alpha_k)} = \dot{x}_k^{(\alpha_k-1)} = \dot{x}_k^{(\alpha_k-1)} \left(x_k, \dot{x}_k, \dots, x_k^{(\alpha_k-1)}, p_{k,\alpha_k-1} \right). \quad (3.42)$$

The remaining conjugate momenta p_{k,β_k-1} for $\beta_k = 1, \dots, (\alpha_k - 1)$ are then determined by the recursion relations (3.37b); it should be stressed, however, that one should not solve these recursion relations for the variables $\dot{x}_k^{(\beta_k-1)}$ in terms of the variables $(x_k, \dot{x}_k, \dots, x_k^{(\beta_k-1)})$, the conjugate momenta $(p_{k,\beta_k}, \dots, p_{k,\alpha_k-2})$, and time derivatives of the latter, since the variables $(x_k, \dot{x}_k, \dots, x_k^{(\alpha_k-1)})$ are regarded as independent in the Ostrogradsky method.

Secondly, the canonical Hamiltonian is defined by equation (3.39), where the velocities $\dot{x}_k^{(\alpha_k-1)}$ have been substituted in accordance with equation (3.42); explicitly it is

$$\begin{aligned} H(x_k^{(\gamma_k)}, p_{k,\gamma_k}) &= \sum_{k=1}^K \dot{x}_k^{(\alpha_k-1)} \left(x_k, \dot{x}_k, \dots, x_k^{(\alpha_k-1)}, p_{k,\alpha_k-1} \right) p_{k,\alpha_k-1} \\ &\quad - L \left(x_k, \dot{x}_k, \dots, x_k^{(\alpha_k-1)}, \dot{x}_k^{(\alpha_k-1)}(\dots) \right) \\ &\quad + \sum_{k=1}^K \sum_{\beta_k=1}^{\alpha_k-1} x_k^{(\beta_k)} p_{k,\beta_k-1}. \end{aligned} \quad (3.43)$$

Eventually it yields Hamilton's equations (3.41), which can be written down—upon the introduction of the fundamental Poisson brackets on the phase space spanned by the pairs of canonically conjugate variables $(x_k^{(\gamma_k)}, p_{k,\gamma_k})$ —as the canonical system

$$\dot{x}_k^{(\gamma_k)} = \{x_k^{(\gamma_k)}, H\}, \quad (3.44a)$$

$$\dot{p}_{k,\gamma_k} = \{p_{k,\gamma_k}, H\}. \quad (3.44b)$$

After the Poisson brackets have been computed, it is necessary to impose the condition that the variables $x_k^{(\gamma_k)}$ be time derivatives of order γ_k of the original coordinates $x_k(t)$. This requirement may be implemented *ab initio* by firstly associating with each variable $x_k^{(\gamma_k)}$ an auxiliary independent degree of freedom; then replacing the original Lagrangian (3.35) by an *extended* Lagrange function, wherein the definitions of the new degrees of freedom in terms of the old ones are inserted as constraints with Lagrange multipliers. It is actually the modern way of building up

an Ostrogradsky formulation and its advantages are twofold. Firstly, it shifts the study of higher-order Lagrangians to the analysis of the usual type of dynamical systems for which powerful techniques have been developed so far (see, for instance [Gov91]); it thus renders the necessity of a separate discussion of the quantisation of higher-order systems void of any justification whatsoever. Moreover the extension of the formalism to embody the case of singular higher-order systems may be done in a natural way along the lines of Dirac's approach (cf. Subsection 3.2.3). Secondly, canonical or path-integral quantisations of such higher-order systems may be achieved unhindered by the possible ambiguity that could arise when dealing with the variables $x_k^{(\gamma_k)}$ and their first-order time derivatives $\dot{x}_k^{(\gamma_k)}$: Without introducing auxiliary degrees of freedom it could indeed be confusing to perform a Legendre transformation on the variables $x_k^{(\alpha_k-1)}$ only, while leaving the other derivatives untouched.

We illustrate the Ostrogradsky construction with a simple example.

Example 3.2.1. We take the Lagrangian $L = \dot{x}^2/2 - \omega^2 x^2/2 - \epsilon^2 \ddot{x}^2/2$ corresponding to a simple (unit-mass) harmonic oscillator with an acceleration-squared term. We firstly consider x and $y := \dot{x}$ as independent variables; the Lagrangian then becomes $L = y^2/2 - \omega^2 x^2/2 - \epsilon^2 \dot{y}^2/2$. We define Ostrogradsky momenta as $p_y := \partial L / \partial \dot{y} = -\epsilon^2 \dot{y}$ and $p_x := \partial L / \partial y - \dot{p}_y = y + \epsilon^2 \ddot{y}$ respectively. Only the former relation is inverted in terms of \dot{y} ; we obtain the Hamiltonian of the system, $H(x, p_x, y, p_y) = y p_x - p_y^2 / 2\epsilon^2 - y^2 / 2 + \omega^2 x^2 / 2$, from which the canonical equations are readily derived: They are $\dot{x} = y$, $\dot{y} = -p_y / \epsilon^2$, $\dot{p}_x = -\omega^2 x$, and $\dot{p}_y = -p_x + y$ respectively. We recognise easily the definitions of y and momenta. Finally we recover the Euler–Lagrange equations from the canonical equations for the momenta, i.e. $\epsilon^2 x^{(4)} + \ddot{x} + \omega^2 x = 0$.

Let us see now how the original Ostrogradsky construction can be treated within the framework of Dirac's Hamiltonian formalism for constrained systems. A separate analysis of regular and singular higher-order systems is at this stage unnecessary for, in both cases, the higher-order Lagrangian is reduced to a first-order Lagrangian exhibiting primary constraints.

3.2.3 Constrained Ostrogradsky construction

Lagrangian formalism

Consider a system with K degrees of freedom x_k for $k = 1, \dots, K$ and assume that the associated Lagrangian (with higher derivatives) be given by expression (3.35). Let us introduce new *independent* variables q_{k,γ_k} for $\gamma_k = 0, \dots, (\alpha_k - 1)$ through

the following recursion relations

$$q_{k,\beta_k} = \dot{q}_{k,\beta_k-1} \quad \text{for } \beta_k = 1, \dots, (\alpha_k - 1), \quad (3.45a)$$

$$q_{k,0} = x_k. \quad (3.45b)$$

Clearly this choice corresponds to assuming that the successive time derivatives $x_k^{(\gamma_k)}$ are specified as independent variables, for relations (3.45) imply

$$q_{k,\gamma_k} \equiv x_k^{(\gamma_k)} \quad \text{for } \gamma_k = 0, \dots, (\alpha_k - 1). \quad (3.46)$$

Preservation of the standard interpretation of the old coordinates when time evolution is considered requires the relations (3.45a) to be brought into the Lagrangian formalism as primary constraints. The initial higher-order Lagrange function L is replaced by an *extended* first-order Lagrangian \underline{L} (with Lagrange multipliers λ_{k,β_k} for $\beta_k = 1, \dots, (\alpha_k - 1)$ as additional variables) that is given by

$$\underline{L}(q_{k,\gamma_k}, \dot{q}_{k,\gamma_k}, \lambda_{k,\beta_k}) := L(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) + \sum_{k=1}^K \sum_{\beta_k=1}^{\alpha_k-1} (q_{k,\beta_k} - \dot{q}_{k,\beta_k-1}) \lambda_{k,\beta_k}. \quad (3.47)$$

The variables $(q_{k,\gamma_k}, \lambda_{k,\beta_k})$ thus encompass the independent degrees of freedom of the extended Lagrangian system, with $(q_{k,\beta_k}, \lambda_{k,\beta_k})$ being *auxiliary* degrees of freedom as compared to the original coordinates $x_k (= q_{k,0})$.

Before resorting to Dirac's analysis we must ensure that both Lagrange functions L and \underline{L} yield equivalent equations of motion [GR94].

Proposition 3.2.1. *Let L be the original Lagrangian (3.35). Let \underline{L} be the associated extended Lagrangian (3.47). The Euler–Lagrange equations corresponding to L and \underline{L} respectively are equivalent.*

Proof. The standard variational principle calls for the action functional constructed from the Lagrangian (3.47) to be stationary under variations of the independent degrees of freedom. With respect to the auxiliary degrees of freedom, it yields the equations

$$[\delta q_{k,\beta_k}] \longrightarrow \frac{\partial L}{\partial q_{k,\beta_k}} + \frac{d}{dt} \lambda_{k,\beta_k+1} + \lambda_{k,\beta_k} = 0 \quad \text{for } \beta_k = 1, \dots, (\alpha_k - 2), \quad (3.48a)$$

$$[\delta q_{k,\alpha_k-1}] \longrightarrow \frac{\partial L}{\partial q_{k,\alpha_k-1}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_{k,\alpha_k-1}} \right) + \lambda_{k,\alpha_k-1} = 0, \quad (3.48b)$$

$$[\delta \lambda_{k,\beta_k}] \longrightarrow q_{k,\beta_k} - \dot{q}_{k,\beta_k-1} = 0, \quad (3.48c)$$

whereas the variation with respect to the original coordinates gives

$$[\delta q_{k,0}] \longrightarrow \frac{\partial L}{\partial q_{k,0}} + \frac{d}{dt} \lambda_{k,1} = 0. \quad (3.48d)$$

These last equations (3.48d) are the actual equations of motion of the system: The former set of equations (3.48a)–(3.48c) contains in fact constraint equations that determine both the auxiliary degrees of freedom q_{k,β_k} as the successive time derivatives of the original coordinates $q_{k,0}$ (equation (3.48c)) and the Lagrange multipliers λ_{k,β_k} in terms of successive partial derivatives of the original Lagrangian L (equations (3.48a) and (3.48b)); we may inject the ensuing multipliers into equations (3.48d) to obtain the equations of motion

$$\sum_{\gamma_k=0}^{\alpha_k-1} (-1)^{\gamma_k} \left(\frac{d}{dt} \right)^{\gamma_k} \frac{\partial L}{\partial q_{k,\gamma_k}} + (-1)^{\alpha_k} \left(\frac{d}{dt} \right)^{\alpha_k} \frac{\partial L}{\partial \dot{q}_{k,\alpha_k-1}} = 0, \quad (3.49)$$

which in turn reduce to the Euler–Lagrange equations (3.36) as soon as we enforce the constraints (3.48c). ■

Remark. Hitherto the procedure has been completely general, that is, irrespective of the regular or singular nature of the original Lagrangian: henceforth we focus the analysis on singular Lagrangians.

Hamiltonian formalism

We now assume that the original higher-order Lagrangian L be singular—though the present analysis applies equally well to regular systems—and that the rank of its associated Hessian matrix be constant everywhere and equal to $K - R$ ($R \in \mathbb{N}$), viz.

$$\text{rank} \left(\frac{\partial^2 L}{\partial x_k^{(\alpha_k)} \partial x_l^{(\alpha_l)}} \right) = \text{rank} \left(\frac{\partial^2 \underline{L}}{\partial \dot{q}_{k,\alpha_k-1} \partial \dot{q}_{l,\alpha_l-1}} \right) = K - R. \quad (3.50)$$

With the aim of developing a Hamiltonian formulation on the basis of the Lagrangian \underline{L} we proceed to the standard Dirac analysis.

The configuration space of the extended system is spanned by the set of variables $(q_{k,\gamma_k}, \lambda_{k,\beta_k})$ for $\gamma_k = 0, \dots, (\alpha_k - 1)$ and $\beta_k = 1, \dots, (\alpha_k - 1)$. We define the momenta canonically conjugate to the independent degrees of freedom as

$$p_{k,\beta_k-1} := \frac{\partial \underline{L}}{\partial \dot{q}_{k,\beta_k-1}} = -\lambda_{k,\beta_k}, \quad (3.51a)$$

$$p_{k,\alpha_k-1} := \frac{\partial \underline{L}}{\partial \dot{q}_{k,\alpha_k-1}} = \frac{\partial L}{\partial \dot{q}_{k,\alpha_k-1}}, \quad (3.51b)$$

$$\pi_{k,\beta_k} := \frac{\partial \underline{L}}{\partial \dot{\lambda}_{k,\beta_k}} = 0, \quad (3.51c)$$

where we have used equation (3.47). We thus see from equations (3.51) that the phase-space degrees of freedom $(q_{k,\gamma_k}, p_{k,\gamma_k}; \lambda_{k,\beta_k}, \pi_{k,\beta_k})$ are not all independent; hence we may identify the following set of primary constraints,

$$\varphi_{k,\beta_k} = p_{k,\beta_k-1} + \lambda_{k,\beta_k} \approx 0, \quad (3.52a)$$

$$\pi_{k,\beta_k} \approx 0, \quad (3.52b)$$

to which we add the constraints stemming from the singular character of the original Lagrangian (cf. equation (3.51b)),

$$\phi_i(q_{k,\gamma_k}, p_{k,\alpha_k-1}) \approx 0 \quad \text{for } i = 1, \dots, R. \quad (3.52c)$$

The first set of primary constraints (3.52a)–(3.52b) originates in the specific way the auxiliary degrees of freedom have been introduced into the extended Lagrange function \underline{L} (cf. equation (3.47)); given the fundamental Poisson brackets on the phase space,

$$\begin{aligned} \{q_{k,\gamma_k}, q_{l,\gamma_l}\} &= 0 = \{p_{k,\gamma_k}, p_{l,\gamma_l}\}, & \{q_{k,\gamma_k}, p_{l,\gamma_l}\} &= \delta_{kl} \delta_{\gamma_k \gamma_l}, \\ \{\lambda_{k,\beta_k}, \lambda_{l,\beta_l}\} &= 0 = \{\pi_{k,\beta_k}, \pi_{l,\beta_l}\}, & \{\lambda_{k,\beta_k}, \pi_{l,\beta_l}\} &= \delta_{kl} \delta_{\beta_k \beta_l}, \end{aligned}$$

these primary constraints satisfy

$$\{\varphi_{k,\beta_k}, \pi_{l,\beta_l}\} = \delta_{kl} \delta_{\beta_k \beta_l} \quad (3.53)$$

and hence are second class (they will be removed from the formalism later on).

Before pursuing Dirac's analysis let us show how it is possible to recover Ostrogradsky's prescriptions for the definition of the momenta p_{k,γ_k} [Pon89].

Proposition 3.2.2. *Let \underline{L} be the extended Lagrangian associated with the original singular Lagrangian L . The Euler–Lagrange equations obtained from \underline{L} with respect to the auxiliary coordinates q_{k,β_k} (for $\beta_k = 1, \dots, \alpha_k - 1$) are equivalent to the recursion relations (3.37) defining the Ostrogradsky momenta p_{k,γ_k} (for $\gamma_k = 0, \dots, \alpha_k - 1$).*

Proof. It is sufficient to examine the Euler–Lagrange equations obtained from the Lagrangian \underline{L} with respect to the auxiliary coordinates q_{k,β_k} , namely

$$\frac{\partial \underline{L}}{\partial q_{k,\beta_k}} - \frac{d}{dt} \left(\frac{\partial \underline{L}}{\partial \dot{q}_{k,\beta_k}} \right) = 0 \quad \text{for } \beta_k = 1, \dots, (\alpha_k - 1). \quad (3.54)$$

Taking definitions (3.47) and constraints (3.52a) into account equations (3.54) are equivalent to

$$p_{k,\beta_k-1} = \frac{\partial L}{\partial q_{k,\beta_k}} - \frac{d}{dt} p_{k,\beta_k} \quad \text{for } \beta_k = 1, \dots, \alpha_k - 1, \quad (3.55)$$

which, owing to the definitions (3.45a) of the auxiliary degrees of freedom, coincide with the recursion relations (3.37b). On the other hand expressions (3.51b) correspond to definition (3.37a). Hence, as announced, we recover the definitions (3.37) of the Ostrogradsky momenta. \blacksquare

Remark. The remaining Euler–Lagrange equations

$$\frac{\partial \underline{L}}{\partial q_{k,0}} - \frac{d}{dt} \left(\frac{\partial \underline{L}}{\partial \dot{q}_{k,0}} \right) = 0 \quad (3.56)$$

are equivalent to the standard Euler–Lagrange equations for the Lagrangian L (cf. equation (3.48d) and the subsequent discussion).

Of particular concern is the prevailing rôle played by the momenta p_{k,α_k-1} : They are indeed the only variables not involved in the primary constraints (3.52a), (3.52b), and their conjugate coordinates q_{k,α_k-1} are the only auxiliary variables the velocities of which do appear in the original Lagrangian L (compare equations (3.51a) with equations (3.51b)). These remarks about the special rôle played by the pairs of conjugate variables $(q_{k,\alpha_k-1}, p_{k,\alpha_k-1})$ motivate the definition of a *restricted* canonical Hamiltonian that gives the energy corresponding to the Lagrangian L when the variables q_{k,β_k-1} for $\beta_k = 1, \dots, (\alpha_k - 1)$ have been frozen; it is

$$H_{\text{r}}(q_{k,\gamma_k}, p_{k,\alpha_k-1}) := \sum_{k=1}^K \dot{q}_{k,\alpha_k-1} p_{k,\alpha_k-1} - L(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \quad (3.57)$$

and dwells in the restricted phase space—irrespective of whether the relations (3.51b) are invertible or not [HRT76, Sun82].

We define the canonical Hamiltonian of the system in accordance with the usual prescription:

$$H_{\text{c}} = \sum_{k=1}^K \sum_{\gamma_k=0}^{\alpha_k-1} \dot{q}_{k,\gamma_k} p_{k,\gamma_k} + \sum_{k=1}^K \sum_{\beta_k=1}^{\alpha_k-1} \dot{\lambda}_{k,\beta_k} \pi_{k,\beta_k} - \underline{L}(q_{k,\gamma_k}, \dot{q}_{k,\gamma_k}, \lambda_{k,\beta_k}). \quad (3.58)$$

Making use of the constraint equations (3.52) and definition (3.57) of the restricted Hamiltonian we may write the canonical Hamiltonian (3.58) as

$$H_{\text{c}}(q_{k,\gamma_k}, p_{k,\gamma_k}) = H_{\text{r}}(q_{k,\gamma_k}, p_{k,\alpha_k-1}) + \sum_{k=1}^K \sum_{\beta_k=1}^{\alpha_k-1} p_{k,\beta_k-1} q_{k,\beta_k}. \quad (3.59)$$

We now proceed to the Dirac analysis of the system the canonical Hamiltonian of which is given by (3.58). Firstly, we write down the Dirac Hamiltonian of the system

$$H_{\text{D}} := H_{\text{c}} + \sum_{k=1}^K \sum_{\beta_k=1}^{\alpha_k-1} \left(\mu^{k,\beta_k} \varphi_{k,\beta_k} + \nu^{k,\beta_k} \pi_{k,\beta_k} \right) + \sum_{i=1}^R \omega^i \phi_i, \quad (3.60)$$

with new Lagrange multipliers μ^{k,β_k} , ν^{k,β_k} , and ω^i associated respectively to the primary constraints (3.52) of the extended system. However, as indicated above, the first two constraints (3.52a) and (3.52b) are second class: They can be removed provided the canonical Poisson bracket is replaced by the appropriate Dirac bracket. Further we can easily check that the consistency algorithm does not generate secondary constraints from these primary ones: Their Dirac bracket with the Dirac Hamiltonian (3.60) must vanish on the constraint surface; this requirement yields a unique determination of the multipliers μ^{k,β_k} and ν^{k,β_k} . We thus solve these second-class constraints, i.e. $\lambda_{k,\beta_k} = -p_{k,\beta_k-1}$ and $\pi_{k,\beta_k} = 0$; hence the Dirac Hamiltonian (3.60) simplifies to

$$H = H_c + \sum_{i=1}^R \omega^i \phi_i. \quad (3.61)$$

The local symplectic structure on the phase space is specified through the fundamental canonical Dirac brackets

$$\{q_{k,\gamma_k}, q_{l,\gamma_l}\}_{\mathcal{D}} = 0 = \{p_{k,\gamma_k}, p_{l,\gamma_l}\}_{\mathcal{D}}, \quad \{q_{k,\gamma_k}, p_{l,\gamma_l}\}_{\mathcal{D}} = \delta_{kl} \delta_{\gamma_k \gamma_l}, \quad (3.62)$$

and time evolution results from the knowledge of this symplectic structure and the explicit form of the Hamiltonian (3.61).

Henceforth we have all the prerequisites at our disposal to generalise Ostrogradsky's theorem for singular Lagrangians [Pon89]; we proceed gradually, establishing partial results which will be collected eventually.

Proposition 3.2.3. *Let H be the Dirac Hamiltonian (3.61) associated with the singular system. The Hamilton–Dirac equations with respect to the variables q_{k,β_k-1} (for $\beta_k = 1, \dots, \alpha_k - 1$) are equivalent to the Lagrangian constraints (3.45a).*

Proof. We readily obtain the equations

$$\dot{q}_{k,\beta_k-1} = \{q_{k,\beta_k-1}, H\}_{\mathcal{D}} = \frac{\partial H}{\partial p_{k,\beta_k-1}} = q_{k,\beta_k}, \quad (3.63)$$

which, obviously, are equivalent to the Lagrangian constraints (3.45a). ■

Proposition 3.2.4. *Let H be the Dirac Hamiltonian (3.61) associated with the singular system. The Hamilton–Dirac equations with respect to the variables q_{k,α_k-1} are equivalent to the definition of the momenta p_{k,α_k-1} .*

Proof. We expand the equations of motion for the variables q_{k,α_k-1} , viz.

$$\begin{aligned}\dot{q}_{k,\alpha_k-1} &= \{q_{k,\alpha_k-1}, H\}_{\mathcal{D}} \\ &= \{q_{k,\alpha_k-1}, H_r\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i \{q_{k,\alpha_k-1}, \phi_i\}_{\mathcal{D}} \\ &= \frac{\partial H_r}{\partial p_{k,\alpha_k-1}} + \sum_{i=1}^R \omega^i \frac{\partial \phi_i}{\partial p_{k,\alpha_k-1}}.\end{aligned}\tag{3.64}$$

These correspond to the first half of Hamilton's equations for the Lagrangian L , where the variables q_{k,β_k-1} have been frozen. Since the functions H_r and ϕ_i depend solely on the momenta p_{k,α_k-1} , the Dirac brackets in (3.64) may be viewed as the canonical brackets defined in the restricted phase space $(q_{k,\alpha_k-1}, p_{k,\alpha_k-1})$. We observe that it is always possible, in principle, to express the multipliers ω^i as functions of the coordinates and velocities $(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1})$ if we solve the equations [Pon89, HT92]

$$\begin{aligned}\dot{q}_{k,\alpha_k-1} &= \frac{\partial H_r}{\partial p_{k,\alpha_k-1}} \left(q_{k,\gamma_k}, p_{k,\alpha_k-1} (q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \right) \\ &\quad + \sum_{i=1}^R \omega^i (q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \frac{\partial \phi_i}{\partial p_{k,\alpha_k-1}} \left(q_{k,\gamma_k}, p_{k,\alpha_k-1} (q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \right),\end{aligned}\tag{3.65}$$

and provided that all the constraints, $\phi_i \approx 0$ for $i = 1, \dots, R$, are independent.⁶ Moreover, the existence of these extra variables ω^i enables us to invert the Legendre transformation defined from (q, \dot{q}) -space to the constraint surface in (q, p, ω) -space by means of the one-to-one correspondence

$$\begin{cases} q_{k,\gamma_k} = q_{k,\gamma_k}, \\ p_{k,\alpha_k-1} = \frac{\partial L}{\partial \dot{q}_{k,\alpha_k-1}}(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}), \\ \omega^i = \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}), \end{cases} \iff \begin{cases} q_{k,\gamma_k} = q_{k,\gamma_k}, \\ \dot{q}_{k,\alpha_k-1} = \frac{\partial H_r}{\partial p_{k,\alpha_k-1}} + \omega^i \frac{\partial \phi_i}{\partial p_{k,\alpha_k-1}}, \\ \phi_i(q_{k,\gamma_k}, p_{k,\alpha_k-1}) = 0. \end{cases}$$

Consequently, equations (3.64) and the definition (3.51b) of the momenta p_{k,α_k-1} are equivalent. ■

Before considering the Hamilton–Dirac equations with respect to the conjugate momenta we can prove the following useful lemma [Pon89].

⁶This corresponds to the *irreducible* case that we assume for simplicity. The reducible case could be treated without much difficulty (see [HT92]).

Lemma 3.2.1. *Under the current assumptions the following identity holds:*

$$\frac{\partial H_r}{\partial q_{k,\gamma_k}} = - \sum_{i=1}^R \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \frac{\partial \phi_i}{\partial q_{k,\gamma_k}} - \frac{\partial L}{\partial q_{k,\gamma_k}}. \quad (3.66)$$

Proof. From the above remarks on the invertible character of the Legendre transformation we may infer the identity

$$\begin{aligned} H_r(q_{k,\gamma_k}, p_{k,\alpha_k-1}(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1})) \\ \equiv \sum_{k=1}^K p_{k,\alpha_k-1}(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \dot{q}_{k,\alpha_k-1} - L(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}), \end{aligned}$$

whence we obtain

$$\frac{\partial H_r}{\partial q_{k,\gamma_k}} = \sum_{l=1}^K \left(\dot{q}_{l,\alpha_l-1} - \frac{\partial H_r}{\partial p_{l,\alpha_l-1}} \right) \frac{\partial p_{l,\alpha_l-1}}{\partial q_{k,\gamma_k}} - \frac{\partial L}{\partial q_{k,\gamma_k}}.$$

After the application of equations (3.65), this becomes

$$\frac{\partial H_r}{\partial q_{k,\gamma_k}} = \sum_{l=1}^K \sum_{i=1}^R \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \frac{\partial \phi_i}{\partial p_{l,\alpha_l-1}} \frac{\partial p_{l,\alpha_l-1}}{\partial q_{k,\gamma_k}} - \frac{\partial L}{\partial q_{k,\gamma_k}}. \quad (3.67)$$

Since the identity

$$\phi_i(q_{k,\gamma_k}, p_{k,\alpha_k-1}(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1})) \equiv 0 \quad (3.68)$$

obviously holds, equation (3.67) reduces to the expected result, namely

$$\frac{\partial H_r}{\partial q_{k,\gamma_k}} = - \sum_{i=1}^R \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \frac{\partial \phi_i}{\partial q_{k,\gamma_k}} - \frac{\partial L}{\partial q_{k,\gamma_k}}. \quad (3.69)$$

■

Consider now the second half of Hamilton's equations.

Proposition 3.2.5. *Let H be the Dirac Hamiltonian (3.61) associated with the singular system. The Hamilton–Dirac equations with respect to the conjugate momenta p_{k,β_k} (for $\beta_k = 1, \dots, \alpha_k - 1$) are equivalent to the Ostrogradsky recursion relations (3.55).*

Proof. We firstly write down the equations of motion with respect to the conjugate momenta p_{k,β_k} :

$$\dot{p}_{k,\beta_k} = \{p_{k,\beta_k}, H\}_{\mathcal{D}} = \{p_{k,\beta_k}, H_r\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i \{p_{k,\beta_k}, \phi_i\}_{\mathcal{D}} - p_{k,\beta_k-1}. \quad (3.70)$$

Owing to Lemma 3.2.1, this reduces to

$$\dot{p}_{k,\beta_k} = \frac{\partial L}{\partial q_{k,\beta_k}} - p_{k,\beta_k-1} \quad \text{for } \beta_k = 1, \dots, \alpha_k - 1, \quad (3.71)$$

which is equivalent to equation (3.55). \blacksquare

We are now at the right stage to prove the Ostrogradsky theorem for constrained systems [Pon89].

Generalised Ostrogradsky theorem. *Let L be a singular Lagrangian depending on generalised coordinates x_k and their time derivatives up to order $\alpha_k \geq 1$ (for $k = 1, \dots, K$). Let \underline{L} be the associated extended Lagrangian depending on the auxiliary degrees of freedom $q_{k,\gamma_k} = x_k^{(\gamma_k)}$ (for $\gamma_k = 0, \dots, \alpha_k - 1$). The Euler–Lagrange equations derived from \underline{L} are equivalent to the system of canonical equations obtained from the Dirac Hamiltonian*

$$H = H_c + \sum_{i=1}^R \omega^i \phi_i.$$

Proof. Owing to Lemma 3.2.1, Hamilton’s equations for the momenta $p_{k,0}$,

$$\dot{p}_{k,0} = \{p_{k,0}, H\}_{\mathcal{D}} = \{p_{k,0}, H_r\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i \{p_{k,0}, \phi_i\}_{\mathcal{D}} - p_{k,\beta_k-1}, \quad (3.72)$$

reduce to

$$\dot{p}_{k,0} = \frac{\partial L}{\partial q_{k,0}}, \quad (3.73)$$

which are identical to the Euler–Lagrange equations (3.38). The conclusion is then readily inferred owing to Proposition 3.2.1, Proposition 3.2.2, Proposition 3.2.3, Proposition 3.2.4, and Proposition 3.2.5. \blacksquare

The above results establish the equivalence between the original Lagrangian equations and Hamilton’s equations derived from the Hamiltonian (3.61). The details of this equivalence are displayed inside the box below.

$\dot{q}_{k,\beta_k-1} = \{q_{k,\beta_k-1}, H\}_{\mathcal{D}}$	\iff	$q_{k,\beta_k} = \dot{q}_{k,\beta_k-1},$ [Lagrangian constraints]
$\dot{q}_{k,\alpha_k-1} = \{q_{k,\alpha_k-1}, H\}_{\mathcal{D}}$	\iff	$p_{k,\alpha_k-1} = \frac{\partial L}{\partial \dot{q}_{k,\alpha_k-1}},$ [Definition of momenta p_{k,α_k-1}]
$\dot{p}_{k,\beta_k} = \{p_{k,\beta_k}, H\}_{\mathcal{D}}$	\iff	$p_{k,\beta_k-1} = \frac{\partial L}{\partial \dot{q}_{k,\beta_k}} - \frac{d}{dt} p_{k,\beta_k},$ [Recursion relations for momenta p_{k,β_k-1}]
$\dot{p}_{k,0} = \{p_{k,0}, H\}_{\mathcal{D}}$	\iff	$\frac{d}{dt} p_{k,0} = \frac{\partial L}{\partial q_{k,0}}.$ [Euler–Lagrange equations]

The canonical equations thus include: Lagrangian constraints corresponding to the auxiliary degrees of freedom; Ostrogradsky's definition of momenta; and the Euler–Lagrange equations of motion.

Remark. If we performed the Legendre transformation on the basis of the definition of momenta (3.37)—that is, without introducing an extended Lagrangian—, then new constraints would arise: Their explicit form would be obtained by requiring that the primary constraints (3.52c) be preserved in time [SSOK89].

If we write down the Hamilton–Dirac equations in the following *nonnormal* form,

$$\frac{dq_{k,\gamma_k}}{dt} = \{q_{k,\gamma_k}, H_c\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \{q_{k,\gamma_k}, \phi_i\}_{\mathcal{D}}, \quad (3.74a)$$

$$\frac{dp_{k,\gamma_k}}{dt} = \{p_{k,\gamma_k}, H_c\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i(q_{k,\gamma_k}, \dot{q}_{k,\alpha_k-1}) \{p_{k,\gamma_k}, \phi_i\}_{\mathcal{D}}, \quad (3.74b)$$

then it is clear that we do not impose any constraint on them—constraints (3.52c) are hidden in equations (3.71). The ability to cast the above equations (3.74) into the standard form

$$\begin{aligned} \frac{dq_{k,\gamma_k}}{dt} &\approx \{q_{k,\gamma_k}, H_c\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i(t) \{q_{k,\gamma_k}, \phi_i\}_{\mathcal{D}}, \\ \frac{dp_{k,\gamma_k}}{dt} &\approx \{p_{k,\gamma_k}, H_c\}_{\mathcal{D}} + \sum_{i=1}^R \omega^i(t) \{p_{k,\gamma_k}, \phi_i\}_{\mathcal{D}}, \end{aligned}$$

where $\omega^i(t)$ are arbitrary functions of time, entails the restriction of the trajectories in phase space to the surface that is generated by the constraints (3.52c). This requirement leads generally to the determination of some multipliers and to secondary constraints as well.

The Hamiltonian formulation of higher-order theories obtained by unifying the Ostrogradsky method with the Dirac formalism for constrained systems is not satisfactory when having in prospect the development of a canonical formalism for gauge theories; the very reason lies in the fact that the usual formulation of gauge theories is given in terms of geometrical quantities like covariant derivatives or curvature tensors: In particular, the prescription (3.45) for introducing the auxiliary degrees of freedom does not take into account any of those features present in a gauge theory. Therefore, we present hereafter in Subsection 3.2.4 a generalisation of the constrained Ostrogradsky construction that will allow us to bring forth a consistent Hamiltonian formulation of higher-order theories of gravity.

Remark on an alternative formalism. A coherent way of building up a Hamiltonian formalism for theories with higher derivatives is provided by the constrained Ostrogradsky method, as explained above. Curiously enough, some authors devised an alternative formalism, in the specific case of second-order gravitational Lagrangians, the peculiarity of which is to preclude the occurrence of constraints at the Lagrangian level [Sch97, Kas97]. The trick is the following: add to the original second-order Lagrangian $L_0(x, \dot{x}, \ddot{x})$ a total time derivative of a second-order arbitrary function $W(x, \dot{x}, \ddot{x})$; replace *straight* into the action functional—that is without Lagrange multipliers—the variables \ddot{x} by new independent degrees of freedom q ; then fix the explicit form of the function W by requiring that variation of the action with respect to q yield precisely the relation $\ddot{x} = q$. This skirting procedure, which takes advantage of the freedom of adding a total derivative to the Lagrangian without altering the equations of motion, is misleading: An ambiguity arises due to the presence of terms involving $d\dot{x}/dt$. For this reason, the would-be advantage of the recipe—the mere absence of constraints in the variational principle—is on the contrary a serious drawback in comparison with the constrained Ostrogradsky approach. Even worst, this contrived formalism comes to naught in the case of *singular* second-order Lagrangians: The treatment of the primary constraints is not compatible with the choice $\ddot{x} = q$ (see the comment on page 82).

3.2.4 Generalised constrained Ostrogradsky construction

The basic idea of the generalised Ostrogradsky method for constrained higher-order systems is to allow for a more general definition of the auxiliary Ostrogradsky variables q_{γ_k} instead of the standard definition (3.46). At first sight the general formalism that is given in the literature provides a satisfactory treatment [BL87, BOS92, GT90]. However, as explained below, it is tainted with a small technical mistake that renders the method ineffective in general; this illustrates how pitfalls may arise when one is building up such an abstract theoretical setting without testing it on simple examples or toy-models. Nevertheless this general formalism can be suitably adapted, taking into account the specific features of the system under investigation; we shall come back to this point later (cf. Subsection 3.3.2 on $f(R)$ theories of gravity); but, in the meantime, we analyse the generalised Ostrogradsky method.

Consider a system with K degrees of freedom x_k for $k = 1, \dots, K$ and assume that the associated Lagrangian (with higher derivatives) be given by expression (3.35). Let us introduce new *independent* variables q_{k, γ_k} for $\gamma_k = 0, \dots, (\alpha_k - 1)$

in accordance with the prescriptions

$$q_{k,\beta_k} = Q_{k,\beta_k}(x_l, \dot{x}_l, \dots, x_l^{(\theta_{kl})}), \quad \theta_{kl} = \min(\beta_k, \alpha_l - 1), \quad (3.75a)$$

$$q_{k,0} = Q_{k,0} = x_k, \quad (3.75b)$$

where Q_{k,β_k} are arbitrary functions that may depend on generalised coordinates x_l and their time derivatives up to order θ_{kl} . We require that relations (3.75a) be invertible in terms of the highest-order time derivatives occurring in the explicit form of the functions Q_{k,β_k} ; this requisite entails the conditions

$$\Delta_\sigma = \det\left(\frac{\partial Q_{k,\sigma}}{\partial x_l^{(\sigma)}}\right) \neq 0 \quad \text{for } \sigma = 1, \dots, N-1, \quad (3.76)$$

where the matrices associated with these nonzero determinants Δ_σ contain only those elements for which the determinant index σ satisfies $\sigma < N (= \sup_k \{\alpha_k\})$ (see Example 3.2.2).

In contrast with the standard definition (3.45) of the auxiliary degrees of freedom, definition (3.75) is more general and it enables one to choose specific forms for the functions Q_{k,β_k} according to the actual characteristics of the system under study. Formally, different choices of functions Q_{k,β_k} will lead to distinct Hamiltonian formulations; in that respect, we will address in the sequel the question of how these various formulations are connected with one another (see Proposition 3.2.8).

We consider now a specific example in order to clarify the practical use of prescriptions (3.75) and (3.76).

Example 3.2.2. Let $L = L(x, \dot{x}, \ddot{x}, x^{(3)}, y, \dot{y}, \ddot{y}, y^{(3)}, y^{(4)})$. We may infer, from the highest-order time derivatives corresponding to x and y occurring in L , the values of α_k , namely $\alpha_x = 3$ and $\alpha_y = 4$ respectively. We introduce new coordinates according to the rules (3.75), that is

$$\begin{aligned} q_{x,0} &= x & q_{y,0} &= y \\ q_{x,1} &= Q_{x,1}(x, \dot{x}, y, \dot{y}) & q_{y,1} &= Q_{y,1}(x, \dot{x}, y, \dot{y}) \\ q_{x,2} &= Q_{x,2}(x, \dot{x}, y, \dot{y}, \ddot{y}) & q_{y,2} &= Q_{y,2}(x, \dot{x}, y, \dot{y}, \ddot{y}) \\ & & q_{y,3} &= Q_{y,3}(x, \dot{x}, y, \dot{y}, \ddot{y}, y^{(3)}). \end{aligned}$$

We then construct the determinants Δ_σ , fulfilling conditions (3.76):

$$\Delta_1 = \begin{vmatrix} \partial Q_{x,1}/\partial \dot{x} & \partial Q_{x,1}/\partial \dot{y} \\ \partial Q_{y,1}/\partial \dot{x} & \partial Q_{y,1}/\partial \dot{y} \end{vmatrix}, \quad \Delta_2 = \begin{vmatrix} \partial Q_{x,2}/\partial \ddot{x} & \partial Q_{x,2}/\partial \ddot{y} \\ \partial Q_{y,2}/\partial \ddot{x} & \partial Q_{y,2}/\partial \ddot{y} \end{vmatrix}, \quad \Delta_3 = \frac{\partial Q_{y,3}}{\partial y^{(3)}}.$$

Owing to conditions (3.76) we may solve equations (3.75a) in terms of time derivatives of order β_k (for $\beta_k = 1, \dots, \alpha_k - 1$) of the generalised coordinates; the resulting functions are

$$x_k^{(\beta_k)} = X_k^{\beta_k}(q_{l,0}, \dots, q_{l,\theta_{kl}}), \quad \det\left(\frac{\partial X_k^\sigma}{\partial q_{l,\sigma}}\right) \neq 0. \quad (3.77)$$

Henceforth we slightly depart from what is found in the literature (see, e.g., [BL87]), wherein an erroneous result renders the subsequent analysis ineffective in general. Nevertheless let us firstly demonstrate the mistake. The authors claim that the first-order time derivatives \dot{q}_{k,β_k-1} could be expressed in terms of the auxiliary degrees of freedom \dot{q}_{l,ρ_l} (for $\rho_l = 0, \dots, \theta_{kl}$) only. However, in general this is not true, for differentiating with respect to time the quantities $x_k^{(\sigma_k)}$ for $\sigma_k = 1, \dots, (\alpha_k - 2)$, which are given in equation (3.77), we obtain the series expansion

$$X_k^{\sigma_k+1} = \sum_{l=1}^K \sum_{\rho_l=0}^{\gamma_{kl}} \frac{\partial X_k^{\sigma_k}}{\partial q_{l,\rho_l}} \dot{q}_{l,\rho_l}, \quad \gamma_{kl} = \min(\sigma_k, \alpha_l - 1), \quad (3.78)$$

which contains explicitly first-derivative terms of the form \dot{q}_{l,α_l-1} if it ever happens that $\sigma_k \geq (\alpha_l - 1)$. Unfortunately this last inequality corresponds to the generic case, as it can more easily be checked on Example 3.2.2. The only means to remove these first-derivative terms is to assume that each coordinate x_k occurring in the Lagrange function L have one and the same maximal order N (i.e. $\alpha_k = N \forall k$). This requirement is not a severe restriction though for we could always add a total derivative term to the original Lagrangian (3.35) without modifying the Lagrangian dynamics and such that the above assumption would be satisfied. However, we must ensure that distinct Hamiltonian formulations stemming from Lagrangians that differ by a total derivative only be equivalent; this is achieved with the following result.⁷

Proposition 3.2.6. *Consider two Lagrangians, L (of order N) and L_0 (of order $N - 1$) that differ by a total time derivative, viz.*

$$L(x, \dot{x}, \dots, x^{(N)}) = L_0(x, \dot{x}, \dots, x^{(N-1)}) + \frac{d}{dt}W(x, \dot{x}, \dots, x^{(N-1)}). \quad (3.79)$$

The two distinct Hamiltonian formulations that are constructed on L and L_0 respectively are canonically equivalent; the appropriate canonical transformation is defined by

$$q_{\beta-1} = q_{\beta-1}^{(0)}, \quad (3.80a)$$

⁷For our purpose it is sufficient to consider only one degree of freedom.

$$p_{\beta-1} = p_{\beta-1}^{(0)} + \frac{\partial W}{\partial q_{\beta-1}^{(0)}}, \quad (3.80b)$$

where $(q_{\beta-1}, p_{\beta-1})$ and $(q_{\beta-1}^{(0)}, p_{\beta-1}^{(0)})$ (for $\beta = 1, \dots, N-1$) denote the canonical variables associated with the Lagrangians L and L_0 respectively.

Proof. We firstly examine the Ostrogradsky formalism for the Lagrangian L_0 . We introduce auxiliary degrees of freedom and their conjugate momenta through the standard recursion relations

$$\begin{aligned} q_0^{(0)} &= x, & p_{N-2}^{(0)} &= \frac{\partial L_0}{\partial \dot{q}_{N-2}^{(0)}}, \\ q_\sigma^{(0)} &= \dot{q}_{\sigma-1}^{(0)}, & p_{\sigma-1}^{(0)} &= \frac{\partial L_0}{\partial q_\sigma^{(0)}} - \frac{d}{dt} p_\sigma^{(0)} \quad \text{for } \sigma = 1, \dots, N-2. \end{aligned}$$

We then obtain the canonical Hamiltonian corresponding to L_0 , namely

$$H_c^{(0)}(q_{\beta-1}^{(0)}, p_{\beta-1}^{(0)}) = \sum_{\sigma=1}^{N-2} q_\sigma^{(0)} p_{\sigma-1}^{(0)} + \dot{q}_{N-2}^{(0)} p_{N-2}^{(0)} - L_0(q_{\beta-1}^{(0)}, \dot{q}_{N-2}^{(0)}).$$

Now we turn to the Ostrogradsky formalism for the Lagrangian L .

Once again we introduce auxiliary degrees of freedom and their conjugate momenta through the standard recursion relations

$$\begin{aligned} q_0 &= x, & p_{N-1} &= \frac{\partial W}{\partial q_{N-1}}, \\ q_\beta &= \dot{q}_{\beta-1}, & p_{\beta-1} &= \frac{\partial L}{\partial q_\beta} - \frac{d}{dt} p_\beta \quad \text{for } \beta = 1, \dots, N-1. \end{aligned}$$

We then obtain the canonical Hamiltonian corresponding to L , namely

$$H_c(q_\gamma, p_\gamma) = \sum_{\beta=1}^{N-1} \left(p_{\beta-1} - \frac{\partial W}{\partial q_{\beta-1}} \right) q_\beta - L_0(q_\gamma) \quad \text{for } \gamma = 0, \dots, N-1.$$

Note that the restricted Hamiltonian (3.57) does not depend here on the momentum p_{N-1} ; hence the pair of canonical variables (q_{N-1}, p_{N-1}) are associated with spurious physical degrees of freedom. It is then straightforward to see that the canonical transformation (3.80) turns the Hamiltonian H_c into the Hamiltonian $H_c^{(0)}$. ■

For completeness we write down the explicit form of the nontrivial primary constraints of the N^{th} -order theory,

$$\phi_{N-1} = p_{N-1} - \frac{\partial W}{\partial q_{N-1}} \approx 0, \quad (3.81a)$$

$$\phi_{N-2} = p_{N-2} - \frac{\partial L_0}{\partial q_{N-1}} - \frac{\partial W}{\partial q_{N-2}} \approx 0. \quad (3.81b)$$

The former constraint is first class and does not generate any secondary constraint; it corresponds to the gauge freedom associated with the choice of the function W , especially with respect to its dependence on the variable q_{N-1} . The last constraint arises from the singular character of the original Lagrangian L_0 ; its preservation in time generates secondary constraints which are classified as usual into first-class and second-class constraints. Furthermore it can be easily shown that the Dirac bracket structure is preserved under the canonical transformation (3.80) and that both Hamiltonian formulations lead to equivalent quantum counterparts via canonical [Kam96] or path-integral quantisation methods [Gro93].

Further remark on an alternative formalism. Proposition 3.2.6 sheds a new light upon the alternative formalism briefly discussed on page 78. Kasper shows that this formalism is canonically equivalent to the Ostrogradsky construction performed on the original second-order Lagrangian L_0 [Kas97]. This relationship is even more manifest when one applies the Ostrogradsky method to the third-order Lagrangian involving the total time derivative of a specific second-order function, the explicit form of which is chosen in accordance with the aforementioned recipe. Indeed, the relation (3.80) enables us to write down the corresponding Ostrogradsky momenta, p_0 and p_1 , in terms of the original momenta, $p_0^{(0)}$ and $p_1^{(0)}$, and compare them with the ‘alternative’ momenta, π_0 and π_1 . We find the relations

$$\begin{aligned} p_0 &= p_0^{(0)} + \frac{\partial W}{\partial q_0^{(0)}} \equiv \pi_0, \\ p_1 &= p_1^{(0)} + \frac{\partial W}{\partial q_1^{(0)}} = \frac{\partial L_0}{\partial \ddot{x}} + \frac{\partial W}{\partial \dot{x}} \equiv 0, \end{aligned}$$

as well as the definition of momentum p_2 ,

$$p_2 = \frac{\partial W}{\partial \ddot{x}} \equiv \pi_1.$$

The vanishing of the momentum p_1 is a direct consequence of the hypothesis that the original Lagrangian be regular and of the condition that has to be fulfilled by the function W to render the alternative formalism meaningful. In other words, the alternative formalism has been defined to preclude the occurrence of the primary constraints (3.81). If the standard constraint analysis is performed within the Ostrogradsky formalism, then the above relations for p_1 and p_2 are second-class constraints.

In agreement with the previous discussion we thus assume that the maximal order of variables x_k is one and the same, that is $\alpha_k = N \forall k$. The auxiliary variables are introduced with the definition (3.75)—with $\theta_{kl} \equiv \beta_k$ —such that conditions (3.76) be fulfilled. Thus, differentiating equations (3.77) with respect to time we can express the time derivative of variables q_{k,β_k-1} as

$$\dot{q}_{k,\beta_k-1} = \mathcal{Q}_{k,\beta_k}(q_{l,0}, \dots, q_{l,\beta_k}), \quad (3.82)$$

where the functions \mathcal{Q}_{k,β_k} can be determined with the recursion relations

$$X_k^1 = \mathcal{Q}_{k,1}, \quad (3.83a)$$

$$X_k^{\sigma_k+1} = \sum_{l=1}^K \sum_{\rho_l=0}^{\sigma_k} \frac{\partial X_k^{\sigma_k}}{\partial q_{l,\rho_l}} \mathcal{Q}_{l,\rho_l+1} \quad \text{for } \sigma_k = 1, \dots, N-2. \quad (3.83b)$$

We introduce *velocities* $v_{k,N-1}$ with the definition

$$v_{k,N-1} := \dot{q}_{k,N-1}. \quad (3.84)$$

Remark. At first sight, it could seem unnecessary to add more degrees of freedom to the theory: Indeed, we did not need to introduce such velocities through the constrained Ostrogradsky construction (cf. Subsection 3.2.3). In the literature the consideration of these new variables is merely a loophole: When one adopts definition (3.84) the equations of motion for the variables $q_{k,N-1}$ simply become Lagrangian constraints; the equivalence with the definition of momenta $p_{k,N-1}$ is lost and primary constraints $\phi_i \approx 0$ do not occur at this stage. So to speak, one eludes the discussion given in the proof of Proposition 3.2.4, that is the discussion on the invertibility of the Legendre transformation associated with the presence of primary constraints $\phi_i \approx 0$. The resulting formalisms are hybrid-like: At one time velocities are regarded as independent degrees of freedom; at another time they are viewed as the first-time derivatives of variables $q_{k,N-1}$. This is confusing and this could lead to mistaken interpretations (see [BL87, BOS92, GT90]). For that very reason we give a more throughout analysis, hereafter.

Assuming that we adopt the definition (3.84) for the velocities $v_{k,N-1}$ we can prove the following result [BL87].

Proposition 3.2.7. *Under the current assumptions the functional form of the highest-order time derivatives of the generalised coordinates x_k is given by*

$$x_k^{(N)} = X_k^N(q_{l,0}, \dots, q_{l,N-1}, v_{l,N-1}), \quad \det\left(\frac{\partial X_k^N}{\partial v_{l,N-1}}\right) \neq 0. \quad (3.85)$$

Proof. Taking into account equations (3.75), (3.77), and (3.82) we obtain successively

$$\begin{aligned} x_k^{(N)} &= \dot{x}_k^{(N-1)} = \sum_{l=1}^K \sum_{\rho_l=0}^{N-1} \frac{\partial X_k^{N-1}}{\partial q_{l,\rho_l}} \dot{q}_{l,\rho_l}, \\ &= \sum_{l=1}^K \sum_{\rho_l=0}^{N-2} \frac{\partial X_k^{N-1}}{\partial q_{l,\rho_l}} \mathcal{Q}_{l,\rho_l+1} + \sum_{l=1}^K \frac{\partial X_k^{N-1}}{\partial q_{l,N-1}} \dot{q}_{l,N-1}, \end{aligned}$$

where the last right-hand side may be written as a function X_k^N , which could be formally given by equation (3.85). \blacksquare

We now interpret equations (3.82) and (3.84) as Lagrangian constraints and we replace the original (higher-order) Lagrange function L by the extended (first-order) Lagrangian \underline{L} ,

$$\begin{aligned} \underline{L}(q, \dot{q}, \lambda, v, \mu) &= L(q, v) + \sum_{k=1}^K \sum_{\beta_k=1}^{N-1} (\dot{q}_{k,\beta_k-1} - \mathcal{Q}_{k,\beta_k}) \lambda_{k,\beta_k} \\ &\quad + \sum_{k=1}^K (\dot{q}_{k,N-1} - v_{k,N-1}) \mu_{k,N-1}, \end{aligned} \quad (3.86)$$

with Lagrange multipliers λ_{k,β_k} and $\mu_{k,N-1}$, so as to recover the interpretation in terms of the original set of coordinates. In close analogy with Proposition 3.2.1 the Euler–Lagrange equations derived from the extended Lagrangian \underline{L} are equivalent to the Euler–Lagrange equations obtained from the original Lagrangian L . (The proof sheds no new light upon the subsequent analysis.)

The momenta canonically conjugate to the independent degrees of freedom are defined respectively by

$$p_{k,\beta_k-1} := \frac{\partial \underline{L}}{\partial \dot{q}_{k,\beta_k-1}} = \lambda_{k,\beta_k}, \quad (3.87a)$$

$$p_{k,N-1} := \frac{\partial \underline{L}}{\partial \dot{q}_{k,N-1}} = \mu_{k,N-1}, \quad (3.87b)$$

$$\pi_{k,\beta_k}^{(\lambda)} := \frac{\partial \underline{L}}{\partial \dot{\lambda}_{k,\beta_k}} = 0, \quad (3.87c)$$

$$\pi_{k,N-1}^{(\mu)} := \frac{\partial \underline{L}}{\partial \dot{\mu}_{k,N-1}} = 0, \quad (3.87d)$$

$$\pi_{k,N-1}^{(v)} := \frac{\partial \underline{L}}{\partial \dot{v}_{k,N-1}} = 0. \quad (3.87e)$$

We thus have five sets of Lagrangian constraints that we denote as $\varphi_{k,\beta_k-1} \approx 0$, $\varphi_{k,N-1} \approx 0$, $\pi_{k,\beta_k}^{(\lambda)} \approx 0$, $\pi_{k,N-1}^{(\mu)} \approx 0$, and $\pi_{k,N-1}^{(v)} \approx 0$ respectively.

The canonical Hamiltonian of the system is readily obtained, viz.

$$H_c(q, p, v) = \sum_{k=1}^K \sum_{\beta_k=1}^{N-1} p_{k,\beta_k-1} \mathcal{Q}_{k,\beta_k} + \sum_{k=1}^K p_{k,N-1} v_{k,N-1} - L(q, v), \quad (3.88)$$

where the constraints in the extended Lagrangian (3.86) have been used.

Before resorting to the Dirac analysis of the system with canonical Hamiltonian (3.88) we must firstly identify the primary constraints that characterise the singular theory under study. In contrast with the standard treatment—the formalism without the extra velocities $v_{k,N-1}$ —, these primary constraints do not occur in definition (3.87b) of the momenta $p_{k,N-1}$. Instead, they occur in the canonical equations of motion for the momenta $\pi^{(v)}$, derived from the canonical Hamiltonian (3.88), viz.

$$\dot{\pi}_{k,N-1}^{(v)} = -\frac{\partial H_c}{\partial v_{k,N-1}} = \frac{\partial L}{\partial v_{k,N-1}} - p_{k,N-1} \approx 0, \quad (3.89)$$

where we have enforced the preservation in time of the constraint (3.87e). In the aforementioned hybrid formalism no rigorous constraint analysis is performed and equation (3.89) is used to define the primary constraints $\phi_i(q, p) \approx 0$. However, if the velocities are considered as independent variables—not merely a handy notation—, then the above interpretation of equation (3.89) is misleading. In other words, to ensure consistency of the formalism one must either refrain oneself from introducing velocities v as additional—though spurious—degrees of freedom or one has to perform the standard constraint analysis, assuming that these velocities are independent—though constrained—degrees of freedom. Choosing the first option we are brought back to the analysis made in Subsection 3.2.3; adopting the second we must consider the Dirac Hamiltonian to be given by

$$\begin{aligned} H_{\mathcal{D}} := H_c &+ \sum_{k=1}^K \sum_{\beta_k=1}^{N-1} \left(\eta^{k,\beta_k-1} \varphi_{k,\beta_k-1} + \xi_{(\lambda)}^{k,\beta_k} \pi_{k,\beta_k}^{(\lambda)} \right) \\ &+ \sum_{k=1}^K \left(\eta^{k,N-1} \varphi_{k,N-1} + \xi_{(\mu)}^{k,N-1} \pi_{k,N-1}^{(\mu)} + \xi_{(v)}^{k,N-1} \pi_{k,N-1}^{(v)} \right), \end{aligned} \quad (3.90)$$

with Lagrange multipliers η and ξ associated with the primary constraints.

Enforcing preservation in time of the primary constraints we obtain

$$\varphi_{k,\beta_k-1} \approx 0 \longrightarrow \xi_{(\lambda)}^{k,\beta_k} = \frac{\partial L}{\partial q_{k,\beta_k-1}} - \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \left(\frac{\partial \mathcal{Q}_{l,\beta_l}}{\partial q_{k,\beta_k-1}} \right) \lambda_{l,\beta_l}, \quad (3.91a)$$

$$\varphi_{k,N-1} \approx 0 \longrightarrow \xi_{(\mu)}^{k,N-1} = \frac{\partial L}{\partial q_{k,N-1}} - \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \left(\frac{\partial \mathcal{Q}_{l,\beta_l}}{\partial q_{k,N-1}} \right) \lambda_{l,\beta_l}, \quad (3.91b)$$

and

$$\pi_{k,\beta_k}^{(\lambda)} \approx 0 \xrightarrow{\cdot} \eta^{k,\beta_k-1} = 0, \quad (3.91c)$$

$$\pi_{k,N-1}^{(\mu)} \approx 0 \xrightarrow{\cdot} \eta^{k,N-1} = 0, \quad (3.91d)$$

$$\pi_{k,N-1}^{(v)} \approx 0 \xrightarrow{\cdot} \chi_{k,N-1}^{(v)} := \frac{\partial L}{\partial v_{k,N-1}} - p_{k,N-1} \approx 0. \quad (3.91e)$$

Some multipliers are thus determined through equations (3.91a)–(3.91d) while the secondary constraints $\chi_{k,N-1}^{(v)}$ do arise from equation (3.91e). Note that all constraints but those associated with the velocities are second class; we can thus coherently remove them from the formalism provided that we define the appropriate Dirac bracket. On the other hand, time-evolution of the secondary constraints $\chi_{k,N-1}^{(v)}$ yields the equation

$$\begin{aligned} \chi_{k,N-1}^{(v)} \approx 0 \xrightarrow{\cdot} & \sum_{l=1}^K \left(\frac{\partial^2 L}{\partial v_{l,N-1} \partial v_{k,N-1}} \right) \xi_{(v)}^{l,N-1} + \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \left(\frac{\partial^2 L}{\partial q_{l,\beta_l-1} \partial v_{k,N-1}} \right) Q_{l,\beta_l} \\ & + \sum_{l=1}^K \left(\frac{\partial^2 L}{\partial q_{l,N-1} \partial q_{k,N-1}} \right) v_{l,N-1} - \xi_{(\mu)}^{k,N-1} = 0, \end{aligned} \quad (3.92)$$

which enables to fix $K - r$ multipliers $\xi_{(v)}$ only, on account of the fact that the rank of the Hessian matrix, as given by equation (3.50), is expressed in terms of the velocities $v_{k,N-1}$ by

$$\text{rank} \left(\frac{\partial^2 L(q, v)}{\partial v_{k,N-1} \partial v_{l,N-1}} \right) = K - r. \quad (3.93)$$

At this stage one may work out the standard consistency algorithm of the Dirac method, ending up eventually with a complete set of primary and secondary constraints, which can be classified into first-class and second-class constraints depending on the specific features of the theory.

Remark. In contradistinction to the hybrid approach [BL87] equation (3.91e) defines constraints, be the system regular or not.

This is now the right stage to address the aforementioned issue on the possible connection between distinct Hamiltonian formulations stemming from different choices of the arbitrary functions Q_{k,β_k} ; the following proposition provides us with the appropriate answer [GT90].

Proposition 3.2.8. *The Hamiltonian formulations developed from one and the same Lagrangian L by different means of introducing the auxiliary degrees of freedom in the generalised Ostrogradsky method are canonically equivalent.*

Proof. It is sufficient to prove that an arbitrary choice of the functions Q_{k,β_k} leads to a Hamiltonian formulation that is canonically equivalent to the constrained Ostrogradsky Hamiltonian formulation of Subsection 3.2.3.

We consider the standard Ostrogradsky variables $(q_{k,\gamma_k}, p_{k,\gamma_k})$ defined as previously by

$$\begin{aligned} q_{k,0} &= x_k, & q_{k,\beta_k} &= x_k^{(\beta_k)}, \\ p_{k,N-1} &= \frac{\partial L}{\partial \dot{q}_{k,N-1}}, & p_{k,\beta_k-1} &= \frac{\partial L}{\partial q_{k,\beta_k}} - \dot{p}_{k,\beta_k}. \end{aligned}$$

We introduce the generalised Ostrogradsky conjugate pairs $(Q_{k,\gamma_k}, P_{k,\gamma_k})$ with the following prescriptions: Firstly, the auxiliary degrees of freedom are defined by

$$\begin{aligned} x_k &= Q_{k,0}, \\ x_k^{(\beta_k)} &= X_k^{\beta_k}(Q_{l,0}, \dots, Q_{l,\beta_k}); \end{aligned}$$

then, their conjugate momenta are determined through the recursion relations

$$\begin{aligned} P_{k,N-1} &= \frac{\partial L}{\partial \dot{Q}_{k,N-1}}, \\ \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \frac{\partial Q_{l,\beta_l}}{\partial Q_{k,\beta_k}} P_{l,\beta_l-1} &= \frac{\partial L}{\partial Q_{k,\beta_k}} - \dot{P}_{k,\beta_k}, \end{aligned}$$

which generalise relations (3.55). (Note that we do not introduce the velocities $v_{k,N-1}$ to keep the comparison between both formalisms more transparent.)

We try to find the generating function of the canonical transformation that maps variables (Q, P) onto variables (q, p) [SM74]. On account of the above definitions of variables q_{k,γ_k} the appropriate choice consists in taking the type-2 generating function $F_2(Q, p)$ that is defined by

$$F_2(Q, p) = \sum_{k=1}^K p_{k,0} Q_{k,0} + \sum_{k=1}^K \sum_{\beta_k=1}^{N-1} p_{k,\beta_k} X_k^{\beta_k}(Q).$$

Indeed, from that specific form we obtain the relationship between variables q_{k,γ_k} and Q_{k,γ_k} , viz.

$$\begin{aligned} q_{k,0} &= \frac{\partial F_2}{\partial p_{k,0}} = Q_{k,0}, \\ q_{k,\beta_k} &= \frac{\partial F_2}{\partial p_{k,\beta_k}} = X_k^{\beta_k}(Q). \end{aligned}$$

On the other hand, the conjugate momenta are transformed as

$$P_{k,0} = \frac{\partial F_2}{\partial Q_{k,0}} = p_{k,0} + \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,0}} p_{l,\beta_l}, \quad (3.94a)$$

$$P_{k,\beta_k} = \frac{\partial F_2}{\partial Q_{k,\beta_k}} = \sum_{l=1}^K \sum_{\beta_l=1}^{N-1} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,\beta_k}} p_{l,\beta_l}. \quad (3.94b)$$

Now we must check that the canonical transformation generated by $F_2(Q, p)$ be preserving the canonical Hamiltonian, viz.

$$H_c(q, p) \equiv H_c(Q, P) \Big|_{Q, P \rightarrow q, p}$$

We start with the canonical Hamiltonian (3.88) obtained in the generalised Ostrogradsky method, namely

$$\begin{aligned} H_c(Q, P) &= \sum_{k=1}^K P_{k,0} \mathcal{Q}_{k,1} + \sum_{k=1}^K \sum_{\sigma_k=1}^{N-2} P_{k,\sigma_k} \mathcal{Q}_{k,\sigma_k+1} \\ &\quad + \sum_{k=1}^K P_{k,N-1} \dot{Q}_{k,N-1} - L(Q, \dot{Q}). \end{aligned}$$

Utilising relation (3.94a) we expand the first term of H_c , which is

$$\sum_{k=1}^K P_{k,0} \mathcal{Q}_{k,1} = \sum_{k=1}^K p_{k,0} \mathcal{Q}_{k,1} + \sum_{k,l=1}^K \sum_{\beta_l=1}^{N-1} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,0}} p_{l,\beta_l} \mathcal{Q}_{k,1}.$$

Making use of relation (3.94b) we find for the second term of H_c the series expansion

$$\sum_{k=1}^K \sum_{\sigma_k=1}^{N-2} P_{k,\sigma_k} \mathcal{Q}_{k,\sigma_k+1} = \sum_{k,l=1}^K \sum_{\beta_l=1}^{N-1} \sum_{\sigma_k=1}^{N-2} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,\sigma_k}} p_{l,\beta_l} \mathcal{Q}_{k,\sigma_k+1}.$$

Repeating once again this procedure for the third term of H_c we obtain

$$\begin{aligned} \sum_{k=1}^K P_{k,N-1} \dot{Q}_{k,N-1} &= \sum_{k,l=1}^K \sum_{\beta_l=1}^{N-1} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,N-1}} p_{l,\beta_l} \dot{Q}_{k,N-1} \\ &= \sum_{k,l=1}^K \frac{\partial X_l^{N-1}}{\partial Q_{k,N-1}} p_{l,N-1} \dot{Q}_{k,N-1}. \end{aligned}$$

In agreement with the proof of Proposition 3.2.7 we derive

$$\dot{q}_k^{(N-1)} = \sum_{l=1}^K \sum_{\rho_l=0}^{N-2} \frac{\partial X_k^{N-1}}{\partial Q_{l,\rho_l}} \mathcal{Q}_{l,\rho_l+1} + \sum_{l=1}^K \frac{\partial X_k^{N-1}}{\partial Q_{l,N-1}} \dot{Q}_{l,N-1},$$

which enables us to rewrite the third term of H_c as

$$\sum_{k=1}^K P_{k,N-1} \dot{Q}_{k,N-1} = \sum_{k=1}^K p_{k,N-1} \dot{q}_{k,N-1} - \sum_{k,l=1}^K \sum_{\rho_l=0}^{N-2} \frac{\partial X_k^{N-1}}{\partial Q_{l,\rho_l}} p_{k,N-1} \mathcal{Q}_{l,\rho_l+1}.$$

Summing up all these intermediate results we obtain for the canonical Hamiltonian H_c the expression

$$\begin{aligned} H_c(Q, P) = & \sum_{k=1}^K p_{k,0} \mathcal{Q}_{k,1} + \sum_{k=1}^K p_{k,N-1} \dot{q}_{k,N-1} - L(q, \dot{q}) \\ & + \sum_{k,l=1}^K \sum_{\beta_l=1}^{N-1} \sum_{\rho_k=0}^{N-2} \frac{\partial X_l^{\beta_l}}{\partial Q_{k,\rho_k}} p_{l,\beta_l} \mathcal{Q}_{k,\rho_k+1} - \sum_{k,l=1}^K \sum_{\rho_l=0}^{N-2} \frac{\partial X_k^{N-1}}{\partial Q_{l,\rho_l}} p_{k,N-1} \mathcal{Q}_{l,\rho_l+1}. \end{aligned}$$

On account of equations (3.83) it is not difficult to show that the last two terms of the above expression simplify to

$$\sum_{k=1}^K \sum_{\sigma_k=1}^{N-2} p_{k,\sigma_k} X_k^{\sigma_k+1}.$$

Hence the canonical Hamiltonian H_c reduces to

$$H_c(q, p) = \sum_{k=1}^K \sum_{\beta_k=1}^{N-1} p_{k,\beta_k-1} q_{\beta_k} + \sum_{k=1}^K p_{k,N-1} \dot{q}_{k,N-1} - L(q, \dot{q}),$$

which coincides with the canonical Hamiltonian (3.59) of the standard Ostrogradsky construction. ■

3.3 Higher-order theories of gravity

3.3.1 A short summary of canonical general relativity

Three-plus-one splitting of space-time

Because general relativity is an already parameterised theory it seems natural to ‘de-parameterise’ it so as to make the constraints manifest and proceed to its canonical formulation (cf. the discussion on page 59). The celebrated path to achieve this programme consists in foliating space-time into three-dimensional spacelike hypersurfaces parameterised by a global time function.⁸ There are, so to speak, two

⁸There are numerous reviews on the 3 + 1-splitting of space-time, which was firstly used in the development of the ADM formalism; one can pick out, e.g., [ADM62, BG70, MTW73, Mac75, Kuc81, Que92].

opposite ways of looking at the reliability of the $3 + 1$ -splitting. The first, which is the most convenient to adopt, advocates its use for any field theory because it yields naturally the determination of the degrees of freedom, the constraints, the gauge freedom, and the field evolution equations [IN80]; in general relativity, in particular, it provides a good insight into the nature of constraints and it simplifies the action principle and the initial-value problem [BG70]. The second point of view stems from the idea that the $3 + 1$ -splitting seems to be contrary to the whole spirit of general relativity. Furthermore this splitting restricts the topology of space-time to be the product of the real line with some three-dimensional manifold. In regard to quantum gravity this inhibition is not welcomed for one would like to allow all possible topologies of space-time [Haw79]. Henceforth we adopt the first, quite conservative, point of view.

The $3 + 1$ -splitting of space-time relies on the following important result (see [Wal84, Chapter 8]).

Theorem 3.3.1. *Let \mathcal{M} be a time-orientable globally hyperbolic space-time endowed with a Lorentzian metric g_{ab} of signature $(-+++)$. Then (\mathcal{M}, g_{ab}) is stably causal. Furthermore a global time function t can be chosen such that each surface of constant t is a Cauchy surface. Thus \mathcal{M} can be foliated by Cauchy surfaces Σ_t and the topology of \mathcal{M} is $\mathbb{R} \times \Sigma$, where Σ denotes any Cauchy surface.*

ADM variables. The basic geometric data of this decomposition are:

- (I) the *intrinsic* geometry of the hypersurfaces Σ_t , described by the induced three-dimensional Riemannian metric h_{ab} on each Σ , which is defined by the formula

$$h_{ab} = g_{ab} + n_a n_b, \quad (3.95)$$

where n^a denotes the unit normal vector field to the hypersurfaces Σ_t (note that h_a^b plays the rôle of a projection operator from the tangent space to \mathcal{M} onto the tangent space to Σ ; $h_a^b : T_P \mathcal{M} \mapsto T_P \Sigma$);

- (II) the way one goes from one hypersurface to the other, determined by the *lapse function* N and the *shift vector* N^a which enable to decompose a ‘time-flow’ vector field t^a on \mathcal{M} satisfying $t^a \nabla_a t = 1$ into its parts normal and tangential to Σ , viz.

$$N = -t^a n_a = \left(n^a \nabla_a t \right)^{-1}, \quad (3.96a)$$

$$N_a = h_{ab} t^b \quad (3.96b)$$

(N measures the rate of flow of proper time with respect to coordinate time as one moves normally to Σ , whereas N^a measures the ‘shift’ tangential to Σ contained in the vector field t^a);

- (III) the way each Σ is embedded in (\mathcal{M}, g_{ab}) , provided by the *extrinsic curvature* tensor K_{ab} which is defined by

$$K_{ab} = -h_a^c h_b^d \nabla_{(c} n_{d)} = -h_b^c \nabla_c n_a = -\frac{1}{2} \mathcal{L}_n h_{ab}, \quad (3.97)$$

where \mathcal{L}_n denotes the Lie derivative along the normal to Σ (one may think of K_{ab} as a generalised notion of time derivative that describes the ‘bending’ of Σ in space-time).

Prescriptions (I-III) above imply that, in terms of N , N^a , and t^a , we have $n^a = (t^a - N^a)/N$ and hence the inverse space-time metric can be written as

$$g^{ab} = h^{ab} - N^{-2} (t^a - N^a) (t^b - N^b). \quad (3.98)$$

This suggests to choose, as the field variables, the spatial metric h_{ab} , the lapse function N , and the covariant shift vector N_a rather than the inverse metric g^{ab} , which is usually used in the variational principle. This equivalent set of variables is usually referred to as ADM *variables*. Furthermore the three-metric h_{ab} uniquely determines the derivative operator on Σ compatible with h_{ab} , which we denote as D_a . Regarding tensor fields on Σ as fields on \mathcal{M} with all their indices orthogonal to n^a we can re-express the action of D_a in terms of that of ∇_a , i.e. the derivative operator associated with g_{ab} , viz.

$$D_c T^{a_1 \dots a_k}_{b_1 \dots b_l} = h^{a_1}_{d_1} \dots h_{b_l}^{e_l} h_c^f \nabla_f T^{d_1 \dots d_k}_{e_1 \dots e_l}. \quad (3.99)$$

The derivative operator D_a brings forth a curvature tensor ${}^{(3)}R^a_{bcd}$ on Σ_t . It is easy to show that, in terms of D_a , the extrinsic curvature tensor in (3.97) takes the form

$$K_{ab} = \frac{1}{2N} (-\mathcal{L}_t h_{ab} + D_a N_b + D_b N_a). \quad (3.100)$$

With respect to a coordinate basis the normal to Σ_t has the components $n^\alpha \equiv (1, -N^i)/N$ and $n_\alpha \equiv (-N, 0)$ respectively and the metric g_{ab} can be cast into the form

$$ds^2 = h_{ij} (dx^i + N^i dt) \otimes (dx^j + N^j dt) - N^2 dt \otimes dt, \quad (3.101)$$

which enables one to identify its components, $g_{\alpha\beta}$, as well as those corresponding to its inverse, $g^{\alpha\beta}$, viz.

$$g_{\alpha\beta} \equiv \begin{pmatrix} N_k N^k - N^2 & N_j \\ N_i & h_{ij} \end{pmatrix}; \quad g^{\alpha\beta} \equiv \frac{1}{N^2} \begin{pmatrix} -1 & N_j \\ N_i & N^2 h^{ij} - N^i N^j \end{pmatrix}. \quad (3.102)$$

We thus see that the covariant components g_{ij} and h_{ij} coincide, whereas the contravariant components g^{ij} and h^{ij} do not. Moreover, with regard to volume elements, we obtain $\sqrt{-g} \equiv N\sqrt{h}$ by application of the Frobenius–Schur formula. In terms of N , N_i , and h_{ij} , the components of the extrinsic curvature tensor defined in (3.97) and (3.100) are given by

$$K_{ij} = \frac{1}{2N} \left(-\frac{\partial h_{ij}}{\partial t} + N_{i|j} + N_{j|i} \right), \quad (3.103)$$

where a vertical stroke denotes covariant differentiation on Σ_t (a semi-colon denotes covariant differentiation in space-time).

The Gauss, Codazzi, and York equations. The space-time curvature tensor R^a_{bcd} is connected with the curvature tensors on Σ , i.e. ${}^{(3)}R^a_{bcd}$ and K_{ab} , through the *Gauss equation*

$${}^{(3)}R^a_{bcd} = h^a_m h_b^f h_c^g h_d^e R^m_{fge} + 2K^a_{[d} K_{c]b}. \quad (3.104)$$

Suitable contractions of this equation with the three-metric h_{ab} yield

$${}^{(3)}R_{ab} = h_a^c h_b^d R_{cd} + n^e n^f h_a^c h_b^d R_{ecfd} + 2K^c_{[b} K_{c]a}. \quad (3.105)$$

In a similar way we derive the *Codazzi equation*

$$h_e^d h_f^c h_g^b n_a R^a_{bcd} = 2D_{[f} K_{e]g}, \quad (3.106)$$

and its contraction,

$$h_c^b n^a R_{ab} = D_c K - D_a K^a_c. \quad (3.107)$$

In addition to the Gauss equation (3.104) and the Codazzi equation (3.106) we derive, after tedious calculations, the *York equation*⁹

$$n^b n^d h_e^a h_f^c R_{abcd} = \mathcal{L}_n K_{ef} + D_{(e} a_{f)} + K_{eg} K^g_f + a_e a_f, \quad (3.108)$$

where a_c stands for the four-acceleration of an observer moving along the normal to Σ , viz. $a_c := n^b \nabla_b n_c$. Note that in the synchronous Gauss system ($N = 1$, $N^i = 0$) equation (3.108) reduces to the most commonly found expression

$$R_{0i0j} = \frac{\partial K_{ij}}{\partial t} + K_{ik} K^k_j, \quad (3.109)$$

⁹It is actually an exercise proposed by York in [MTW73]; a detailed proof can be found in [Que92].

on account of the following formula expressing the Lie derivative of K_{ij}

$$\mathcal{L}_n K_{ij} = \frac{1}{N} \left(\frac{\partial K_{ij}}{\partial t} - N^k K_{ij|k} - N^k_{|i} K_{kj} - N^k_{|j} K_{ik} \right). \quad (3.110)$$

Contraction of the York equation (3.108) readily yields

$$n^a n^b R_{ab} = h^{ab} \mathcal{L}_n K_{ab} + h^{ab} D_{(a} a_{b)} + K_{ab} K^{ab} + a_c a^c. \quad (3.111)$$

Making use of the contracted Gauss equation (3.105) and the contracted York equation (3.111) we obtain a general expression for the scalar curvature, viz.

$$R = {}^{(3)}R + K^2 - 3K_{ab} K^{ab} - 2h^{ab} \mathcal{L}_n K_{ab} - 2h^{ab} D_{(a} a_{b)} - 2a_c a^c. \quad (3.112)$$

From equations (3.111) and (3.112) we obtain

$$2n^a n^b G_{ab} = {}^{(3)}R + K^2 - K_{ab} K^{ab}. \quad (3.113)$$

Hence setting the left-hand side in equations (3.113) and (3.107) to zero we find the initial-value constraint equations of general relativity in vacuum.

For completeness we may write the Codazzi equation (3.106) and the York equation (3.108) in terms of the Weyl tensor, viz.

$$h_e^d h_f^c h_g^b n_a C_{bcd} = 2 \left[h_e^d h_f^c h_g^b - \frac{1}{2} h^{bd} (h_{eg} h_f^c - h_{fg} h_e^c) \right] D_{[c} K_{d]b}, \quad (3.114a)$$

$$\begin{aligned} n^b n^d h_e^a h_f^c C_{abcd} &= \frac{1}{2} (h_e^a h_f^c - \frac{1}{3} h_{ef} h^{ac}) \\ &\quad \times (\mathcal{L}_n K_{ac} + {}^{(3)}R_{ac} + K K_{ac} + D_{(a} a_{c)} + a_a a_c). \end{aligned} \quad (3.114b)$$

We can specialise the Gauss, Codazzi, and York equations (3.104), (3.106), and (3.108), which are pure tensorial expressions, to the ADM basis, which is defined by $\{\vec{e}_n = (\partial_t - N^i \partial_i)/N, \vec{e}_i = \partial_i\}$. We obtain respectively

$$R^l_{ijk} = {}^{(3)}R^l_{ijk} + K_{ik} K^l_j - K_{ij} K^l_k, \quad (3.115a)$$

$$R^n_{ijk} = K_{ij|k} - K_{ik|j}, \quad (3.115b)$$

$$R_{ninj} = \mathcal{L}_n K_{ij} + \frac{N_{|ij}}{N} + K_{ik} K^k_j. \quad (3.115c)$$

The set of equations (3.115) does provide all the information that is necessary to express the components of any four-dimensional curvature tensor in terms of the intrinsic and extrinsic three-dimensional tensors and of the lapse function and shift

vector. For instance, the components of the Einstein tensor are given by

$$\begin{aligned} G_{nn} &= \frac{1}{2}({}^{(3)}R + K^2 - K_{ij}K^{ij}), \\ G_{nk} &= K_{|k} - K^j_{k|j}, \\ G_{kl} &= {}^{(3)}G_{kl} + KK_{kl} - 2K_{ki}K^i_l - \frac{1}{2}h_{kl}(K^2 - 3K_{ij}K^{ij}) \\ &\quad + (h_{kl}h^{ij} - \delta_k^i\delta_l^j)\mathcal{L}_n K_{ij} + \frac{1}{N}(h_{kl}h^{ij}N_{ij} - N_{kl}). \end{aligned}$$

On the other hand, equation (3.112) for the scalar curvature reduces to

$$R = {}^{(3)}R + K^2 - 3K_{ij}K^{ij} - 2N^{-1}h^{ij}N_{ij} - 2h^{ij}\mathcal{L}_n K_{ij}. \quad (3.116)$$

ADM gravitational Hamiltonian—Surface terms

In most field theories the Hamiltonian can be derived from the covariant action in a systematic way. In general relativity the situation is more intricate due to the presence of a surface term in the Einstein–Hilbert action. This difficulty was not addressed by Arnowitt, Deser, and Misner (ADM) who conducted the first major investigation into general relativity—conceived as a dynamical system [AD59, ADM59, ADM60, ADM62]. Although they highlighted the importance of the constraints and showed that the Hamiltonian is precisely the spatial integral of the constraints, they inadvertently discarded a total derivative term inherently present in the gravitational action. By contrast, DeWitt was the first to realise that the identification of the Hamiltonian with the constraints is only valid in the case when the three-manifold is compact, without boundaries [DeW67]; in the case where the three-manifold is open, boundary conditions become crucial. Consider for instance the asymptotically flat situation: DeWitt put the total derivative term—which becomes a surface term at spatial infinity—back into the Hamiltonian and recovered the fact that the value of the Hamiltonian at a solution coincides with the ADM energy. Further investigation by Regge and Teitelboim demonstrated that the ‘correct’ boundary conditions, together with the requirement that the Hamiltonian and its variations be well defined, lead to the existence of ten surface integrals—the Poincaré charges—in the Hamiltonian of the theory, which are connected with the Poincaré group of transformations acting at spatial infinity [RT74, HRT76]. Beig and ó Murchadha further re-examined this formulation in the language of symplectic geometry (they also corrected a mistake in Regge–Teitelboim’s work having to do with the generator of boosts) [BóM87].

On the other hand, Gibbons and Hawking have advocated the addition *ad hoc* to the Einstein–Hilbert action of the surface integral $2\oint K d\Sigma$, the explicit form of which was firstly determined by York in a different context [Yor72], where K is the

trace of the extrinsic curvature of the boundary [GH77]. There are two separate arguments requiring that this boundary term be added to the Einstein–Hilbert action. In the first argument, one demands that the solutions of the classical field equations be extrema of the action under all perturbations that vanish on the boundary, i.e. $\delta h_{ab} = 0$ on $\partial\mathcal{M}$. This means that, on the boundary, only the normal derivatives of the induced metric are allowed to vary. In order to satisfy this condition one has to add a compensating term to the action the virtue of which is to cancel the second-order derivatives of the metric present in the scalar curvature. This compensating term is precisely the surface integral of the trace of the extrinsic curvature. The second argument, which entails the same boundary term, is formulated in the context of the path-integral formulation of the theory [Haw79, Haw93]: The gravitational action must be such that the amplitude to go from an initial to a final hypersurface must be independent of any arbitrary intermediate hypersurfaces and their associated induced three-metrics.

Hawking and Horowitz have recently re-examined this long-standing discussion on surface integrals for manifolds with boundaries [HH96a].¹⁰ Starting from the Einstein–Hilbert action they derive the gravitational Hamiltonian without discarding any surface term—in contrast with the prevalent procedure. In particular, they show that the boundary terms in the Hamiltonian come directly from the boundary terms in the action and do not need to be added ‘by hand’. They generalise the definition of the ADM energy for space-times that are not asymptotically flat though asymptotically approaching a static background solution. (They also discuss the effect of horizons and the relation between their area and the total entropy of black holes.) We follow their approach.

We start with the gravitational action in vacuum,

$$S[g] = \frac{1}{16\pi} \int_{\mathcal{M}} \sqrt{-g} R - \frac{1}{8\pi} \oint_{\partial\mathcal{M}} d\Sigma K, \quad (3.117)$$

where K is the trace of the extrinsic curvature of the boundary and $d\Sigma$ is the surface element. (We assume that the boundary $\partial\mathcal{M}$ consists of an initial and final surface with unit normal n^a , and a surface near infinity Σ^∞ , with unit normal r^a , on which n^a is tangent.) As indicated above, the surface term in the action (3.117) is required so that the variational principle yield the correct equations of motion subject only to the condition that the induced three-metric on the boundary be held fixed—see, e.g., [Wal84, Appendix E], the specific works of Charap and Nelson [CN83], and York’s [Yor88] (and references therein). Note that the action (3.117) is well defined for spatially compact geometries only—e.g., closed cosmological

¹⁰See also Hawking and Hunter’s generalisation in the presence of nonorthogonal boundaries [HH96b].

models.¹¹

Pure divergences are hidden in equation (3.112): We derive an expression of the scalar curvature where they appear explicitly. We firstly have

$$R = 2(G_{ab} - R_{ab})n^a n^b. \quad (3.118)$$

The first term in equation (3.118) is given by equation (3.113) whereas the second term can be evaluated from the definition of the Riemann tensor given on page 6 with $u^a \equiv n^a$, viz.

$$n^a n^b R_{ab} = K^2 - K_{ab}K^{ab} - \nabla_a(n^a \nabla_b n^b) + \nabla_b(n^a \nabla_a n^b). \quad (3.119)$$

Hence the scalar curvature is given by the general expression

$$\begin{aligned} R &= {}^{(3)}R - K^2 + K_{ab}K^{ab} + 2[\nabla_a(n^a \nabla_b n^b) - \nabla_b(n^a \nabla_a n^b)] \\ &= {}^{(3)}R - K^2 + K_{ab}K^{ab} - 2\nabla_c(Kn^c + a^c), \end{aligned} \quad (3.120)$$

which is equivalent to equation (3.112). Observe that in the ADM basis the volume integral of the four-divergence $\nabla_c(Kn^c)$ contributes the term $\partial_n(\sqrt{h}K)$ to the action whereas in a coordinate basis it yields $\partial_t(\sqrt{h}K) - \sqrt{h}(KN^k)_{|k}$; in the latter case, adding the four-divergence $\nabla_c a^c$ we recover the expression first given by DeWitt [DeW67], namely $-2\partial_t(\sqrt{h}K) + 2\sqrt{h}(KN^k - N^{[k})_{|k}$.

When substituted into the action (3.117) the two total derivative terms in equation (3.120) give rise to boundary contributions according to the formula

$$\int_{\mathcal{M}} d^4x \sqrt{-g} \nabla_a A^a = \int_{\mathcal{M}} d^4x \partial_a [\sqrt{-g} A^a] = \oint_{\partial\mathcal{M}} d\sigma_a A^a, \quad (3.121)$$

where the surface element $d\sigma_a$ is defined by $d\sigma_a = \nu_a d\Sigma = \epsilon \nu_a \sqrt{|h|} d^3x$, where ν^a is the unit normal to the boundary and $\epsilon = \nu^a \nu_a$ ($\epsilon = -1$ or $+1$ whether ν^a is timelike or spacelike respectively). As indicated above, the explicit form of the surface integral was first written down by York in his analysis of canonical gravity based on the ADM decomposition of space-time [Yor72]. The first total divergence in (3.120) neatly cancels the $\oint K$ surface term on the initial and final boundaries: We have indeed $-2 \int_{\mathcal{M}} d^4x \sqrt{-g} \nabla_c(Kn^c) = -2 \oint d^3x \sqrt{h} K$. The second, which is orthogonal to the normal n^a , only contributes to the surface integral near infinity¹²

¹¹For noncompact geometries one must choose a *reference background* which is required to be a static solution to the field equations. The physical action is then the difference between the original action and the action that is evaluated on this background (see [GH93, HH96a] for a foolproof analysis).

¹²The boundary near infinity, denoted by Σ^∞ , is foliated by a family of two-surfaces S_t^∞ coming from its intersection with Σ_t .

and is therefore only relevant for noncompact geometries. This surface integral also contains the contribution from the $\oint K$ surface term in the action (3.117); explicitly it is

$$\frac{1}{8\pi} \oint_{\Sigma^\infty} \sqrt{|h|} (\nabla_c r^c - r_c a^c) = \frac{1}{8\pi} \oint_{\Sigma^\infty} \sqrt{|h|} (g^{ab} + n^a n^b) \nabla_a r_b, \quad (3.122)$$

where r^c denotes the unit normal to Σ^∞ . Hence the action (3.117) takes the form

$$S[h] = \int N dt \left[\frac{1}{16\pi} \int_{\Sigma_t} \sqrt{h} \left({}^{(3)}R + K_{ab} K^{ab} - K^2 \right) - \frac{1}{8\pi} \oint_{S_t^\infty} \sqrt{|h|} {}^{(2)}K \right], \quad (3.123)$$

where ${}^{(2)}K$ is the two-dimensional extrinsic curvature of S_t^∞ in Σ_t .

We thus take as the gravitational Lagrangian density

$$\mathfrak{L}[N, N^i, h_{ij}] = \frac{N\sqrt{h}}{16\pi} \left({}^{(3)}R + K_{ij} K^{ij} - K^2 \right) \quad (3.124)$$

and introduce the canonical momenta Π , Π_i , and π_{ADM}^{ij} conjugate to N , N^i , and h_{ij} respectively, namely¹³

$$\Pi = \frac{\delta \mathfrak{L}}{\delta(\partial_t N)} = 0, \quad (3.125a)$$

$$\Pi_i = \frac{\delta \mathfrak{L}}{\delta(\partial_t N^i)} = 0, \quad (3.125b)$$

$$\pi_{\text{ADM}}^{ij} = \frac{\delta \mathfrak{L}}{\delta(\partial_t h_{ij})} = -\frac{\sqrt{h}}{16\pi} (K^{ij} - K h^{ij}). \quad (3.125c)$$

The action (3.123) can be brought to canonical form by means of the usual procedure, viz.

$$S = \int dt \left[\int_{\Sigma_t} \left(\pi_{\text{ADM}}^{ij} \partial_t h_{ij} - N \mathcal{H} - N^i \mathcal{H}_i \right) - \frac{1}{8\pi} \oint_{S_t^\infty} \left(N \sqrt{|h|} {}^{(2)}K + N_i \pi_{\text{ADM}}^{ij} r_j \right) \right], \quad (3.126)$$

where we have introduced the following quantities

$$\mathcal{H} = 16\pi G_{ijkl} \pi_{\text{ADM}}^{ij} \pi_{\text{ADM}}^{kl} - \frac{\sqrt{h}}{16\pi} {}^{(3)}R, \quad (3.127a)$$

$$\mathcal{H}^i = -2\pi_{\text{ADM}}^{ij} |_{,j}, \quad (3.127b)$$

¹³Since N and N^i are cyclic variables, they have no dynamics—their conjugate momenta vanish identically. They can be considered just as Lagrange multipliers rather than phase-space variables. (This feature of the gravitational Lagrangian can be traced back to the diffeomorphism-invariance of general relativity.)

and the so-called *DeWitt metric*,

$$G_{ijkl} = \frac{1}{2\sqrt{h}}(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}), \quad (3.127c)$$

and where an additional surface term stemming from the Legendre transformation has been taken into account. The canonical Hamiltonian is thus

$$H_c = \int_{\Sigma_t} \left(N\mathcal{H} + N^i\mathcal{H}_i \right) + \frac{1}{8\pi} \oint_{S_t^\infty} \left(N\sqrt{|h|} {}^{(2)}K + N_i \pi_{\text{ADM}}^{ij} r_j \right). \quad (3.128)$$

This expression diverges in general. However, once the Hamiltonian for the reference background has been obtained, one can define the total energy of a given stationary solution of the field equations to be simply the value of the *physical* Hamiltonian,

$$E = \frac{1}{8\pi} \oint_{S_t^\infty} \left[N\sqrt{|h|} \left({}^{(2)}K - {}^{(2)}K_0 \right) + N_i \pi_{\text{ADM}}^{ij} r_j \right], \quad (3.129)$$

where the subscript ‘0’ refers to the background solution. This expression, firstly obtained by Hawking and Horowitz, generalises the famous ADM energy for asymptotically flat space-times [HH96a].

Remark. As indicated above, surface terms play a crucial rôle for noncompact geometries—they cannot be discarded. Another difficulty which arises with surface terms has to do with spatially homogeneous cosmologies: genuine Lagrangian and Hamiltonian formulations are lacking for class B models (see [Mac75] and references therein). This is because the very symmetries that are imposed prevent the boundary terms to be vanishing; hence the equations derived from symmetry-preserving variations are the wrong equations. (We re-examine this issue in greater detail in Subsection 4.1.2.)

Canonical quantisation—Wheeler–DeWitt equation. From equation (3.125) we see that there are primary constraints, $\Pi \approx 0$ and $\Pi_i \approx 0$; their complete treatment was performed by Dirac, DeWitt, and others—this is discussed in several textbooks (see, e.g., [Hel80, Esp92]).

Requiring the preservation in time of the primary constraints one finds as secondary constraints the *super-Hamiltonian*, $\mathcal{H} \approx 0$, and *super-momentum*, $\mathcal{H}_i \approx 0$. (The consistency algorithm does not lead to any new constraints.) For compact geometries the total Hamiltonian is thus given by

$$H_T = \int_{\Sigma_t} \left(N\mathcal{H} + N^i\mathcal{H}_i + \mu\Pi + \mu^i\Pi_i \right), \quad (3.130)$$

where μ and μ^i are Lagrange multipliers. All the constraints are first class: The super-Hamiltonian \mathcal{H} is responsible for the dynamics whereas the super-momenta \mathcal{H}_i are the generators of spatial coordinate transformations on Σ_t . Strictly speaking, the constraints $\mathcal{H}_i \approx 0$ express that the state of the universe depends only on the intrinsic three-geometry of the spatial sections and not on the coordinates. (This leads naturally to the concept of *Wheeler's superspace* [Whe64].)

In conformity with the canonical formulation it is clear that Einstein's equations can be split into two sets: the dynamical equations and the initial-value equations. The former are the evolution equations for the dynamical variables h_{ij} and π_{ADM}^{ij} ; these cannot be freely specified on a given hypersurface Σ_t owing to the constraints, which constitute the second set of initial-value equations. Both groups of equations are intimately connected. Actually, the initial-value equations contain all the dynamics of the gravitational field so that one could say that Einstein's equations are highly redundant. Solving the constraints and fixing the gauge—i.e. picking up a specific coordinate system—one removes four degrees of freedom out of the six pairs of canonical variables; hence the number of physical degrees of freedom is two, which correspond to the two helicity states of the spin-2 graviton.

There are at least three distinct methods to proceed to the canonical quantisation of general relativity: the ADM procedure in which all the constraints are solved and the gauge is fixed before quantising (reduced formalism); the Dirac *modus operandi* in which the constraints are imposed as restrictions on the quantum state of the universe; and an intermediate approach devised by Kuchař [Kuc72]. In all these approaches the quantum state of the system is represented by a wave functional $\Psi[h_{ij}]$ —a functional on Wheeler's superspace. An important feature of this wave function, which appears when one considers closed cosmological models—the basic assumption of quantum cosmology; see [Hal91]—, is that it does not depend explicitly on the coordinate time label t (as a direct consequence of the vanishing of the super-Hamiltonian).

According to the Dirac quantisation method the wave function is annihilated by the operator versions of the (first-class) classical constraints: The usual substitutions for the momenta having been made, viz.

$$\pi_{\text{ADM}}^{ij} \rightarrow -i \frac{\delta}{\delta h_{ij}}, \quad (3.131)$$

one obtains the following equations for Ψ ,¹⁴

$$\mathcal{H}_k \Psi = 2i D_l \frac{\delta \Psi}{\delta h_{kl}} = 0 \quad [\text{momentum constraint}], \quad (3.132a)$$

¹⁴We do not address here the operator-ordering issue.

$$\mathcal{H}\Psi = \left[-16\pi G_{ijkl} \frac{\delta}{\delta h_{ij}} \frac{\delta}{\delta h_{kl}} - \frac{\sqrt{h}}{16\pi} {}^{(3)}R \right] \Psi = 0 \quad [\text{Wheeler-DeWitt equation}]. \quad (3.132b)$$

The momentum constraint (3.132a) is nothing but the quantum mechanical expression of the invariance of the theory under three-dimensional diffeomorphisms. The Wheeler-DeWitt equation (3.132b) is a second-order hyperbolic functional differential equation describing the dynamical evolution of the wave equation in superspace; it must be supplemented by appropriate boundary conditions.

Remark. As an alternative to the canonical quantisation procedure one can construct the wave function using a path-integral approach (see, e.g., [Hal91, Haw93] and references therein).

3.3.2 Hamiltonian formulation of nonlinear gravity theories

Consider the Lagrangian density describing nonlinear theories of gravity, namely

$$\mathfrak{L} = \sqrt{-g} f(R), \quad \text{with } f'' \neq 0, \quad (3.133)$$

where $f(R)$ is a nonlinear arbitrary smooth function of the scalar curvature and primes denote differentiation with respect to the scalar curvature.

We assume that the space-time is foliated into three-dimensional Cauchy hypersurfaces Σ_t and we adopt the ADM basis (cf. 3 + 1-splitting, on page 89). On account of the explicit form (3.116) of the scalar curvature in terms of the intrinsic geometry and extrinsic three-curvature tensor K_{ij} on Σ_t and according to the definition (3.97) of K_{ij} in terms of the Lie derivative of the three-metric h_{ij} along the normal to Σ_t , we may rewrite the Lagrangian density (3.133) as

$$\mathfrak{L} = N\sqrt{h} f\left(R(h_{ij}, \mathcal{L}_n h_{ij}, \mathcal{L}_n^2 h_{ij})\right). \quad (3.134)$$

Since the lapse function N and shift vector N^i are not dynamical variables, we regard them merely as Lagrange multipliers associated with the gravitational constraints. Furthermore we interpret the Lie derivative along the normal to Σ_t as a generalised notion of time differentiation.¹⁵ We follow the generalised constrained Ostrogradsky construction developed in Subsection 3.2.4 in order to cast the theory into canonical form.

Remark. Very recently, Ezawa et al. have performed a similar analysis of the nonlinear Lagrangian density (3.133) [EKK⁺98]. They obtain comparable results albeit utilising a slightly different Hamiltonian formulation: They intimately follow the

¹⁵To bear in mind this interpretation and to make the comparison with the general formalism easier we sometimes use a dot as an alternative notation for the Lie derivative.

generalised Ostrogradsky method referred to as Buchbinder–Lyakhovich’s method. Strictly speaking, they introduce velocities with the definition (3.84) (as indicated above, cf. the remark made on page 83, such an adjunction is unnecessary); they treat N and N^i as genuine canonical variables; and they use the partial time derivative ∂_t instead of the generalised notion of time differentiation provided by the Lie derivative \mathcal{L}_n along the normal to Σ_t . In contrast with their approach the method presented here is more straightforward and clear-cut.

In regard to the second-order Lagrangian density (3.134) the generalised Ostrogradsky prescriptions (3.75) entail the following natural choice for the auxiliary field variables:

$$q_{0,ij} := h_{ij}, \quad (3.135a)$$

$$q_{1,ij} := Q_{1,ij}(h_{ij}, \mathcal{L}_n h_{ij}) = K_{ij}, \quad (3.135b)$$

$$\dot{q}_{1,ij} := \mathcal{L}_n K_{ij}. \quad (3.135c)$$

Owing to the definition (3.135b), conditions (3.76) are automatically fulfilled since equation (3.77) becomes

$$\mathcal{L}_n h_{ij} \equiv \dot{q}_{0,ij} = -2q_{1,ij}, \quad (3.136)$$

which actually corresponds to equation (3.82).

The extended Lagrangian density that includes the above Lagrangian constraint (3.136) supersedes the original Lagrangian density (3.134); it is given by

$$\underline{\mathcal{L}}(q_0, q_1, \dot{q}_0, \dot{q}_1, \lambda) = N^{-1} \mathcal{L}(q_0, q_1, \dot{q}_1) + (\dot{q}_{0,ij} + 2q_{1,ij}) \lambda^{ij}, \quad (3.137)$$

with suitable Lagrange multipliers λ^{ij} so as to recover the interpretation in terms of the original set of field variables. (Observe that an overall N has been factorised.)

The momenta canonically conjugate to the field variables are defined respectively by

$$p_0^{ij} = p^{ij} := \frac{\partial \underline{\mathcal{L}}}{\partial \dot{q}_{0,ij}} = \lambda^{ij}, \quad (3.138a)$$

$$p_1^{ij} = \mathcal{P}^{ij} := \frac{\partial \underline{\mathcal{L}}}{\partial \dot{q}_{1,ij}} = N^{-1} \frac{\partial \mathcal{L}}{\partial (\mathcal{L}_n K_{ij})} = -2\sqrt{h} h^{ij} f'(R), \quad (3.138b)$$

$$\Pi_{ij}^{(\lambda)} := \frac{\partial \underline{\mathcal{L}}}{\partial \dot{\lambda}^{ij}} = 0. \quad (3.138c)$$

Hence we have the primary constraints

$$\varphi^{ij} = p^{ij} - \lambda^{ij} \approx 0, \quad (3.139a)$$

$$\phi^{ij}(q_0, q_1, p_1) = \mathcal{P}^{ij} \approx 0, \quad (3.139b)$$

$$\Pi_{ij}^{(\lambda)} \approx 0, \quad (3.139c)$$

where $\mathcal{P}^{\text{T}ij}$ is the traceless part of \mathcal{P}^{ij} . The constraint (3.139b) arises from the indeterminacy of $(\mathcal{L}_n K_{ij})^{\text{T}}$ in the definition of momenta (3.138b).

Now we perform a restricted Legendre transformation. From equations (3.116) and (3.138b) we obtain

$$\dot{q}_{1,ij} p_1^{ij} = \mathcal{P}^{ij} \mathcal{L}_n K_{ij} = -\frac{\mathcal{P}}{6} \left(R - {}^{(3)}R + 3K_{ij} K^{ij} - K^2 + 2N^{-1} h^{ij} N_{|ij} \right). \quad (3.140)$$

The last term in equation (3.140) gives rise to the surface integral at spatial infinity¹⁶

$$\frac{1}{3} \oint_{\Sigma^\infty} d^3x \left(\mathcal{P} N^{|k} - N \mathcal{P}^{|k} \right) r_k, \quad (3.141)$$

which, in general, does not vanish for noncompact geometries. Henceforth we assume that we are dealing with actions that do not produce such nonzero surface terms. (We shall come back to this specific issue in the study of spatially homogeneous cosmologies within the Hamiltonian framework, in Subsection 4.1.2.) The surface term (3.141) is the only one arising in the theory, in contradistinction to canonical general relativity, where the additional boundary term $\partial_n(\sqrt{h} K)$ must be cancelled out by the Gibbons–Hawking’s compensating boundary term.

The restricted Hamiltonian density is

$$\begin{aligned} \mathfrak{H}_r(h, K, \mathcal{P}) &= \mathcal{P}^{ij} \mathcal{L}_n K_{ij} - N^{-1} \mathfrak{L}(R) \\ &= \frac{\mathcal{P}}{6} \left({}^{(3)}R - 3K_{ij} K^{ij} + K^2 \right) - \frac{1}{3} h^{ij} \mathcal{P}_{|ij} + V(\mathcal{P}), \end{aligned} \quad (3.142)$$

where the ‘potential term’

$$V(\mathcal{P}) := \sqrt{h} \left[R f'(R) - f(R) \right]_{R \rightarrow F(\mathcal{P})} \quad (3.143)$$

has been introduced—upon eliminating R for $F(\mathcal{P})$, the function that is obtained by solving the trace of equation (3.138b) for the trace of the momentum \mathcal{P}^{ij} .

The canonical Hamiltonian density is given by

$$\mathfrak{H}_c(h, K, p, \mathcal{P}) = \mathfrak{H}_r(h, K, \mathcal{P}) - 2p^{ij} K_{ij}. \quad (3.144)$$

Therefore, the Hamiltonian form of the gravitational action based on the original Lagrangian density (3.133) can be written, up to boundary terms, as

$$S = \int_{\mathcal{M}} N \left[p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} - \mathfrak{H}_c(h, K, p, \mathcal{P}) \right]. \quad (3.145)$$

¹⁶We keep the same notations as those used in the discussion on the boundary terms present in the gravitational action; pp. 94 ff.

The ensuing Dirac Hamiltonian density is

$$\mathfrak{H}_{\mathcal{D}} = N\mathcal{H} + N^k\mathcal{H}_k + \mu_{kl}\varphi^{kl} + \nu^{kl}\Pi_{kl}^{(\lambda)} + \xi_{kl}\phi^{kl}. \quad (3.146)$$

Preservation in time of the primary constraints (3.139) leads to the secondary constraints

$$\chi^{ij} = 2p^{\text{T}ij} + \frac{1}{3}\mathcal{P}K^{\text{T}ij} \approx 0 \quad (3.147)$$

and enables to determine the Lagrange multipliers μ_{ij} , ν^{ij} , and ξ_{ij} . Aside from the usual super-Hamiltonian and super-momentum constraints, which are always first class, all other constraints are second class by virtue of the Poisson brackets

$$\{\varphi^{ij}(\mathbf{x}), \Pi_{kl}^{(\lambda)}(\mathbf{y})\} = -\delta_k^i\delta_l^j\delta(\mathbf{x}-\mathbf{y}), \quad (3.148a)$$

$$\{\phi^{ij}(\mathbf{x}), \chi^{kl}(\mathbf{y})\} = \frac{\mathcal{P}}{3}(h^{ik}h^{jl} - \frac{1}{3}h^{ij}h^{kl})\delta(\mathbf{x}-\mathbf{y}). \quad (3.148b)$$

Therefore, we regard them as strong equations provided we introduce the appropriate Dirac bracket.

Expressing the Lie derivative in terms of the usual time derivative we recover the familiar form of the canonical action, namely

$$S = \int_{\mathcal{M}} \left(p^{ij} \dot{h}_{ij} + \mathcal{P}^{ij} \dot{K}_{ij} - N\mathcal{H} - N^k\mathcal{H}_k \right), \quad (3.149)$$

where the super-Hamiltonian and super-momentum constraints are given respectively by

$$\mathcal{H} = \frac{\mathcal{P}}{6} \left({}^{(3)}R - 3K_{ij}K^{ij} + K^2 \right) + V(\mathcal{P}) - \frac{1}{3}h^{ij}\mathcal{P}_{|ij} - 2p^{ij}K_{ij}, \quad (3.150a)$$

$$\mathcal{H}_k = \frac{\mathcal{P}}{3}K_{|k} - \frac{2}{3}(\mathcal{P}K_k^j)_{|j} - 2h_{ik}p^{ij}_{|j}. \quad (3.150b)$$

Counting the number of physical degrees of freedom is straightforward: Once the constraints have been enforced and some coordinate system has been chosen, there remains only three pairs of independent canonical variables. This is in total agreement with the particle content of the theory and with the fact that nonlinear theories of gravity are dynamically equivalent to scalar-tensor theories (cf. Section 2.3). We proceed now to a deeper analysis on this last property in the light of the Hamiltonian formalism.

Dynamical equivalence with scalar-tensor theories

Nothing whatsoever can prevent us from introducing a scalar field, Φ , as a new independent degree of freedom, by adopting, instead of the nonlinear Lagrangian

density (3.133), the equivalent constrained Lagrangian density

$$\mathfrak{L} = \sqrt{-g} \left[f(\Phi) + f'(\Phi)(R - \Phi) \right], \quad (3.151)$$

which is sometimes referred to as a *Helmholtz* Lagrangian density.

According to the Ostrogradsky prescriptions, we define the auxiliary variables

$$\begin{aligned} q_{0,ij} &= h_{ij}, & q_{0,\Phi} &= \Phi, \\ q_{1,ij} &= K_{ij}, & \dot{q}_{0,\Phi} &= \mathcal{L}_n \Phi, \\ \dot{q}_{1,ij} &= \mathcal{L}_n K_{ij}, \end{aligned}$$

and replace the original Lagrangian density (3.151) by the extended one,

$$\underline{\mathfrak{L}}(q_0, q_1, \dot{q}_0, \dot{q}_1, \Phi, \lambda) = N^{-1} \mathfrak{L}(q_0, q_1, \dot{q}_1, \Phi) + (\dot{q}_{0,ij} + 2q_{1,ij}) \lambda^{ij}. \quad (3.152)$$

The conjugate momenta are given by (3.138) and $\Pi^{(\Phi)} = 0$. In addition to the primary constraints (3.139) we also obtain

$$\begin{aligned} \Xi &= \mathcal{P} + 6\sqrt{h}f'(\Phi) \approx 0, \\ \Pi^{(\Phi)} &\approx 0. \end{aligned}$$

The Dirac Hamiltonian density is

$$\mathfrak{H}_{\mathcal{D}} = \mathfrak{H}_{\text{c}} + \mu_{kl} \varphi^{kl} + \nu^{kl} \Pi_{kl}^{(\lambda)} + \xi_{kl} \phi^{kl} + \zeta \Xi + \eta \Pi^{(\Phi)}, \quad (3.153)$$

where the canonical Hamiltonian density is given by

$$\mathfrak{H}_{\text{c}} = \frac{\mathcal{P}}{6} {}^{(3)}R - \frac{\mathcal{P}}{2} K_{ij} K^{ij} + \frac{\mathcal{P}}{6} K^2 - \frac{1}{3} h^{ij} \mathcal{P}_{|ij} + V(\Phi) - 2p^{ij} K_{ij}, \quad (3.154)$$

with a ‘potential term’

$$V(\Phi) := \sqrt{h} \left[\Phi f'(\Phi) - f(\Phi) \right]. \quad (3.155)$$

Time evolution of the primary constraints yields the determination of the Lagrange multipliers and produces the secondary constraint (3.147). All constraints are second class; we can readily eliminate the spurious degrees of freedom associated with λ and Φ from the action, bearing in mind that the function $f'(\Phi)$ has to be inverted. The outcome of this procedure is precisely the canonical formalism that was developed for the Lagrangian density (3.133), where the variable \mathcal{P} plays the rôle of the new independent scalar degree of freedom.

Extended gravity theories

The Ostrogradsky method is also well suited for building up a canonical formalism of theories derived from Lagrangians that are functions not only of the scalar curvature R but also $\square^n R$ (such terms can be generated by quantum corrections to general relativity). The resulting theories, called generically *extended gravity theories*, have been studied in the context of inflationary cosmology; in particular, Wands has discussed their relationship with scalar-tensor theories [Wan94] (see also Section 2.3).

Consider, for instance, the Lagrangian density that describes sixth-order gravity, namely

$$\mathfrak{L} = \sqrt{-g} \left(R + \gamma R \square R \right), \quad (3.156)$$

which is dynamically equivalent to the scalar-tensor Lagrangian density (with two scalar fields)

$$\mathfrak{L} = \sqrt{-g} \left[R(1 + \gamma\varphi_1 + \gamma\square\varphi_0) - \gamma\varphi_0\varphi_1 \right]. \quad (3.157)$$

We may define the auxiliary Ostrogradsky variables

$$\begin{aligned} q_{0,ij} &= h_{ij}, & \varphi_0^{(0)} &= \varphi_0, \\ q_{1,ij} &= K_{ij}, & \varphi_1^{(0)} &= \mathcal{L}_n \varphi_0, \\ \dot{q}_{1,ij} &= \mathcal{L}_n K_{ij}, & \dot{\varphi}_1^{(0)} &= \mathcal{L}_n^2 \varphi_0, \end{aligned}$$

and replace the original Lagrangian density (3.157) by the extended one

$$\begin{aligned} h^{-1/2} \underline{\mathfrak{L}} &= R(q_0, q_1, \dot{q}_1) \left\{ 1 + \gamma \left(\varphi_1 - \dot{\varphi}_1^{(0)} \right) + \gamma q_0^{kl} \left[\varphi_{0|kl}^{(0)} + N^{-1} N_{|k} \varphi_{0|l}^{(0)} \right] \right\} \\ &\quad - \gamma \varphi_0^{(0)} \varphi_1 + \lambda^{ij} (\dot{q}_{0,ij} + 2q_{1,ij}) + \mu \left(\dot{\varphi}_0^{(0)} - \varphi_1^{(0)} \right), \end{aligned}$$

where we have used the useful formula

$$\square\phi = h^{ab} D_a D_b \phi - \mathcal{L}_n^2 \phi + a^c \partial_c \phi.$$

Then we may proceed in the same way as in the nonlinear $f(R)$ case. (We do not elaborate further on this example since the procedure is systematic—although the ensuing expressions are very awkward.)

3.3.3 Link between the Ostrogradsky and ADM formulations of Einstein's theory

Ostrogradsky–ADM equivalence theorem

Now that—as a direct application of the generalised constrained Ostrogradsky construction—we have achieved a consistent Hamiltonian formulation of nonlinear

theories of gravity, it is of great interest to examine whether this method could likewise be used on the *linear* Lagrangian of general relativity. This prospect arose in connection with the problem of determining appropriate boundary conditions in a theory of gravity with higher derivatives. We have seen on page 102 that the only boundary term in the nonlinear case is a surface integral at spatial infinity. This can be easily understood since there is no need whatsoever to discard a total divergence that embodies second-order derivatives of the metric: The Ostrogradsky method is inherently appropriate to cope with higher derivatives. If one could treat—as we surmise—general relativity within the Ostrogradsky scheme, then exactly the same argument would apply: No boundary terms other than the analogue of the surface integral (3.141) would arise. What would then be the relationship between the Ostrogradsky formalism and the ADM version of canonical gravity? We intend, in this subsection, to unravel that possible connection.

Our starting point is the Einstein–Hilbert Lagrangian density,

$$\mathfrak{L} = \sqrt{-g} R. \quad (3.158)$$

We rely on what we did in the previous subsection since the linear Lagrangian density (3.158) may be viewed as a special instance of the nonlinear theory, provided we relax the condition on the second derivative of the function $f(R)$, that is $f'' = 0$.

Instead of utilising expression (3.120) of the scalar curvature as in the ADM method, we exploit the formula (3.116). Thus we can formally rewrite the Lagrangian density (3.158) as

$$\mathfrak{L} = N\sqrt{h} R(h_{ij}, \mathcal{L}_n h_{ij}, \mathcal{L}_n^2 h_{ij}). \quad (3.159)$$

Following the prescriptions of the generalised Ostrogradsky construction we introduce the auxiliary variables (3.135) together with the Lagrangian constraint (3.136) and we replace the original Lagrangian density (3.159) by the appropriate extended Lagrangian density with Lagrange multipliers λ^{ij} .

The momenta canonically conjugate to the field variables are given by equations (3.138), where $f'(R) = 1$, that is $p^{ij} = \lambda^{ij}$, $\mathcal{P}^{ij} = -2\sqrt{h} h^{ij}$, and $\Pi_{ij}^{(\lambda)} = 0$. We thus obtain the primary constraints

$$\varphi^{ij} = p^{ij} - \lambda^{ij} \approx 0, \quad (3.160a)$$

$$\phi^{ij} = \mathcal{P}^{ij} \approx 0, \quad (3.160b)$$

$$\Xi = \mathcal{P} + 6\sqrt{h} \approx 0, \quad (3.160c)$$

$$\Pi_{ij}^{(\lambda)} \approx 0. \quad (3.160d)$$

(Note that the definition (3.138b) of the momenta p_1^{ij} is now a primary constraint since $f'(R) = 1$.)

Performing a Legendre transformation we obtain the canonical Hamiltonian density,

$$\mathfrak{H}_c(h, K, p, \mathcal{P}) = \frac{\mathcal{P}}{6} \left({}^{(3)}R - 3K_{ij}K^{ij} + K^2 \right) - 2p^{ij}K_{ij}, \quad (3.161)$$

and a surface integral at spatial infinity,

$$-2 \oint_{\Sigma^\infty} d\sigma_k N^{|k}, \quad (3.162)$$

which can also be derived straightly by setting $\mathcal{P} = -6\sqrt{h}$ in the expression (3.141). The Dirac Hamiltonian density of the system is given by

$$\mathfrak{H}_\mathcal{D} = \mathfrak{H}_c + \mu_{kl}\varphi^{kl} + \nu^{kl}\Pi_{kl}^{(\lambda)} + \xi_{kl}\phi^{kl} + \zeta\Xi. \quad (3.163)$$

Preservation in time of the primary constraints (3.160) produces the secondary constraints

$$\chi^{ij} = 2p^{ij} + \frac{1}{3}\mathcal{P}K^{ij} \approx 0 \quad (3.164)$$

and enables one to determine all the Lagrange multipliers. All constraints are second class; we can impose them as strong equations in the action, provided we define the appropriate Dirac bracket. We now demonstrate that the reduction process that consists in eliminating all the second-class constraints leads to the ADM form of the canonical action.

Ostrogradsky–ADM equivalence theorem. *The action of general relativity in the ‘Ostrogradsky-Hamiltonian’ form*

$$S_{\text{OSTRO}} = \int dt \left[\int_{\Sigma_t} N \left(p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} - \mathfrak{H}_c(h, K, p, \mathcal{P}) \right) - \frac{1}{8\pi} \oint_{S_t^\infty} \sqrt{|h|} (r_j N^{|j}) \right], \quad (3.165)$$

with the canonical Hamiltonian density given by equation (3.161), coincides exactly, after all the second-class constraints have been solved, with the ADM action of general relativity (without the ad hoc compensating boundary term $\oint K$),

$$S_{\text{ADM}} = \int dt \left[\int_{\Sigma_t} \left(\pi_{\text{ADM}}^{ij} \partial_t h_{ij} - N\mathcal{H} - N^i \mathcal{H}_i - 2\partial_n(\sqrt{h}K) \right) - \frac{1}{8\pi} \oint_{S_t^\infty} \left(r_j (\sqrt{|h|} N^{|j} + N_i \pi_{\text{ADM}}^{ij}) \right) \right], \quad (3.166)$$

with the super-Hamiltonian and super-momentum defined by (3.127).

Proof. Firstly, we expand the ‘ $p\dot{q}$ ’ terms in the Ostrogradsky action (3.165), making use of formulæ (3.103) and (3.110), viz.

$$\begin{aligned} N \left[p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} \right] &= p^{ij} \partial_t h_{ij} - 2p^{ij} N_{i|j} + \mathcal{P}^{ij} \partial_t K_{ij} \\ &\quad - \mathcal{P}^{ij} \left(N^k K_{ij|k} + 2N^k_{|i} K_{jk} \right). \end{aligned}$$

Solving the second-class constraints amounts to eliminating variables \mathcal{P}^{ij} and K_{ij} according to the strong equations

$$\mathcal{P}^{ij} \equiv -2\sqrt{h} h^{ij}, \quad p^{ij} \equiv \sqrt{h} K^{ij}.$$

Hence we obtain successively

$$\begin{aligned} p^{ij} \partial_t h_{ij} + \mathcal{P}^{ij} \partial_t K_{ij} &= (-p^{ij} + p h^{ij}) \partial_t h_{ij} - 2\partial_t (\sqrt{h} K) \\ &= \pi_{\text{ADM}}^{ij} \partial_t h_{ij} - 2\partial_t (\sqrt{h} K), \end{aligned}$$

and

$$\begin{aligned} -2p^{ij} N_{i|j} - \mathcal{P}^{ij} \left(N^k K_{ij|k} + 2N^k_{|i} K_{jk} \right) &= 2 \left(p^{ij} N_{i|j} + N^i p_{|i} \right) \\ &= 2(p^{ij} N_i)_{|j} + 2N_i \pi_{\text{ADM}}^{ij}{}_{|j}. \end{aligned}$$

Summing up the above results we have

$$\begin{aligned} N \left[p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} \right] &= \pi_{\text{ADM}}^{ij} \partial_t h_{ij} - 2\partial_n (\sqrt{h} K) \\ &\quad - 2(\pi_{\text{ADM}}^{ij} N_i)_{|j} + 2N_i \pi_{\text{ADM}}^{ij}{}_{|j}, \end{aligned}$$

where we have utilised the identity

$$2\partial_t (\sqrt{h} K) - 2(p^{ij} N_i)_{|j} \equiv 2\partial_n (\sqrt{h} K) + 2(\pi_{\text{ADM}}^{ij} N_i)_{|j}.$$

The term $-2(\pi_{\text{ADM}}^{ij} N_i)_{|j}$ yields the surface integral at spatial infinity in the ADM action (3.166), i.e.

$$-\frac{1}{8\pi} \oint_{S_t^\infty} \left(r_j \pi_{\text{ADM}}^{ij} N_i \right);$$

the term $2N_i \pi_{\text{ADM}}^{ij}{}_{|j}$ gives the ADM super-momentum (3.127b).

Now we examine the Ostrogradsky canonical Hamiltonian density in (3.165). We readily obtain from equation (3.161) the expression

$$\mathfrak{H}_c(h, K, p, \mathcal{P}) \equiv -\sqrt{h} {}^{(3)}R + \frac{1}{\sqrt{h}} \left(\pi_{\text{ADM}}^{ij} \pi_{ij}^{\text{ADM}} - \frac{1}{2} \pi_{\text{ADM}}^2 \right),$$

which obviously coincides with the ADM super-Hamiltonian (3.127b). ■

Boundary terms in the light of the Ostrogradsky approach

The equivalence of the Ostrogradsky and ADM canonical versions of the gravitational action of general relativity sheds a new light upon the question of boundary terms in the gravitational action. We can regard the Einstein–Hilbert action as a limiting case of the nonlinear gravitational action when $f(R) \equiv R$. In the latter case the only boundary term is the surface integral (3.141). The arguments that lead to the adjunction of the compensating term $2\oint K d\Sigma$ in the Einstein–Hilbert action come to naught in the higher-order case.¹⁷

Firstly, there is no need whatsoever to eliminate the second-order derivatives of the metric. The Ostrogradsky construction of Subsection 3.3.2 shows that the configuration space is spanned by the induced metric and the trace of the extrinsic curvature. As a consequence, no compensating boundary terms are required to cancel surface integrals involving the latter quantity: The variation of K vanishes on the boundary $\partial\mathcal{M}$.¹⁸

Secondly, consider a transition from an initial configuration $(h_{ab}^{(1)}, K^{(1)})$ on a hypersurface Σ_1 to a configuration $(h_{ab}^{(2)}, K^{(2)})$ on an intermediate hypersurface Σ_2 , then followed by a transition to a final configuration $(h_{ab}^{(3)}, K^{(3)})$ on a hypersurface Σ_3 . As indicated above (on page 95), in a consistent path-integral formulation of the theory one expects that the amplitude to go from the initial to the final configuration should be obtained by integrating over all configurations on the intermediate hypersurface Σ_2 . This amounts to require

$$S[g_{ab}^{(I)} + g_{ab}^{(II)}] = S[g_{ab}^{(I)}] + S[g_{ab}^{(II)}], \quad (3.167)$$

where $g_{ab}^{(I)}$ is the metric between Σ_1 and Σ_2 , which induces $(h_{ab}^{(1)}, K_{ab}^{(1)})$ on Σ_1 and $(h_{ab}^{(2)}, K^{(2)})$ on Σ_2 ; $g_{ab}^{(II)}$ is the metric between Σ_2 and Σ_3 , which induces $(h_{ab}^{(2)}, K^{(2)})$ on Σ_2 and $(h_{ab}^{(3)}, K^{(3)})$ on Σ_3 ; and $g_{ab}^{(I)} + g_{ab}^{(II)}$ is the metric obtained by joining together the two regions. In general relativity the three-metrics induced on the intermediate hypersurface Σ_2 by $g_{ab}^{(I)}$ and $g_{ab}^{(II)}$ agree; but the extrinsic curvatures need not: this results in a δ -function in the Ricci curvature of $g_{ab}^{(I)} + g_{ab}^{(II)}$ of strength given by the difference of the extrinsic curvatures on Σ_2 [Haw79]. In the nonlinear case the fact that the respective traces of the extrinsic curvature tensors are one and the same on Σ_2 is sufficient to remove the difficulty: This is fairly confirmed by

¹⁷This was firstly argued by Horowitz in the context of Euclidean quantum gravity with a positive-definite action containing quadratic curvature terms [Hor85] (see also the similar work of Barth, where the Euler characteristic class for the manifold is taken into account [Bar85]). As this applies to the nonlinear case as well, we take up Horowitz's line of thought hereafter.

¹⁸In general relativity imposing that δK be zero on the boundary is strictly forbidden since this would overdetermine the theory.

the explicit computation of the boundary variation of the nonlinear action [MB89], viz.

$$\delta S|_{\partial\mathcal{M}} = 2 \oint_{\partial\mathcal{M}} f' \delta K. \quad (3.168)$$

It is not, in general, possible to write the right-hand side of equation (3.168) as the variation on the boundary of a functional, as is the case in general relativity; the only circumstances under which this programme can effectively been achieved are when the space-time manifold is maximally symmetric [MB89]. As a matter of fact, according to the discussion above on the crucial rôle of K , the right-hand side of equation (3.168) actually vanishes: The possible compensating term is reduced to naught.

Furthermore, when passing from the nonlinear case to the linear Einstein–Hilbert action, one clearly sees how the boundary term $2 \oint K d\Sigma$ materialises: The trace K becomes a spurious degree of freedom and thereby cannot be held fixed any longer on the boundary.

3.3.4 Hamiltonian formulation of quadratic theories of gravity

In the introduction of Section 3.2 on page 61 we have reviewed the works inspired by the Ostrogradsky method, with regard to the canonical formulation of higher-order theories of gravity. In addition, there are two major contributions dealing with quadratic theories of gravity that do not explicitly resort to the Ostrogradsky construction. Both of them require the reduction of the theory to a first-order form. To achieve this end Safko and Elston examined the connection between the Lagrange multiplier approach, thoroughly analysed in Section 2.2, and the ADM formalism [SE76]. They pointed out that there is a sharp difference between the constrained Palatini variational method and the Lagrange multiplier method that they used to cast higher-order curvature invariants into canonical form. Applying an ‘Ostrogradsky-like’ constrained formalism they succeeded—at least formally—in formulating a canonical version of the pure R^2 theory. We are indebted to Boulware for the second contribution, in which he has undertaken the quantisation programme of quadratic gravity and has addressed a certain number of technical and physical issues arising when higher derivatives are present in a (gravitational) field theory [Bou84]. In contrast with Buchbinder and Lyakhovich’s systematic approach (cf. page 63), Boulware’s *modus operandi* seems quite heuristic at first glance. (However, in our opinion this is still the best reference with respect to canonical quadratic gravity.) One advantage of Boulware’s formalism lies in its extensive use of the Lie derivative—instead of time differentiation—which appreciably simplifies the technicalities; this contrasts with Buchbinder and Lyakhovich’s

formalism, which is—in that respect—quite difficult to decipher.

In this subsection we rely on the generalised constrained Ostrogradsky scheme, which was thoroughly analysed in Subsection 3.2.4 and already applied successfully to nonlinear gravity theories in Subsection 3.3.2: We intend to cast the generic quadratic gravitational action into Hamiltonian form.

Remark. The approach given here differs slightly from Boulware’s as well as Buchbinder and Lyakhovich’s treatments in the way we set it up. It is perhaps more transparent in regard to the Ostrogradsky method. The three methods lead to the same results, eventually.

The generic quadratic theory. We consider the most general quadratic Lagrangian density in a four-dimensional space-time (\mathcal{M}, g_{ab}) ,

$$\mathcal{L} = \sqrt{-g} \left(\Lambda + \frac{1}{2\kappa^2} R - \frac{\alpha}{4} C_{abcd} C^{abcd} + \frac{\beta}{8} R^2 \right), \quad (3.169)$$

where Λ is the cosmological constant, $\kappa^2 = 8\pi G_N$, and α, β are dimensionless coupling constants.

Remark. Owing to the Gauss–Bonnet or Lanczos topological invariant in four dimensions, we could equally have chosen $\mu R_{ab} R^{ab} + \nu R^2$ as the relevant quadratic Lorentz-invariant combination in the Lagrangian density, with $\mu = -\alpha/2$ and $\nu = \beta/8 + \alpha/6$. However—it is just a matter of convenience—the choice exhibited in equation (3.169) is more appropriate for discussing the particular variants of the general theory.

As usual we assume that space-time is foliated into three-dimensional Cauchy hypersurfaces Σ_t and we adopt the ADM basis (cf. the 3 + 1-splitting on page 89). We recall here the expression (3.116) of the scalar curvature, viz.

$$R = {}^{(3)}R + K^2 - 3K_{ij}K^{ij} - 2N^{-1}h^{ij}N_{|ij} - 2h^{ij}\mathcal{L}_n K_{ij}, \quad (3.170)$$

and we specialise formulæ (3.114) to the ADM basis, viz.

$$C^{\mathbf{n}}_{ijk} = \left[\delta_i^r \delta_j^s \delta_k^t - \frac{1}{2} h^{rt} (h_{ik} \delta_j^s - h_{ij} \delta_k^s) \right] (K_{rs|t} - K_{rt|s}), \quad (3.171a)$$

$$C_{\mathbf{n}ij} = \frac{1}{2} (\delta_i^k \delta_j^l - \frac{1}{3} h_{ij} h^{kl}) (\mathcal{L}_n K_{kl} + N^{-1} N_{|kl} + K K_{kl} + {}^{(3)}R_{kl}). \quad (3.171b)$$

Since the Weyl tensor identically vanishes in three dimensions, the quadratic Weyl invariant $C_{abcd}C^{abcd}$ reduces to

$$C_{abcd}C^{abcd} = 4(2C_{\mathbf{n}ij}C^{\mathbf{n}ij} + C_{\mathbf{n}ijk}C^{\mathbf{n}ijk}), \quad (3.172)$$

where the explicit forms of $C_{\mathbf{n}ijk}$ and $C_{\mathbf{n}ij}$ are displayed in equations (3.171) above.

As in the nonlinear case (cf. Subsection 3.3.2), we regard the Lagrangian density (3.169) as a functional of the three-metric and its successive Lie derivatives, namely $\mathfrak{L}(h_{ij}, \mathcal{L}_n h_{ij}, \mathcal{L}_n^2 h_{ij})$; we then introduce Ostrogradsky auxiliary variables according to the same prescriptions as given by equations (3.135); we replace the original Lagrangian density (3.169) by an extended one, i.e. $\underline{\mathfrak{L}}$, and define the canonically conjugate momenta:

$$p^{ij} := \frac{\partial \underline{\mathfrak{L}}}{\partial \mathcal{L}_n h_{ij}} = \lambda^{ij}, \quad (3.173a)$$

$$\mathcal{P}^{ij} := \frac{\partial \underline{\mathfrak{L}}}{\partial \mathcal{L}_n K_{ij}} = N^{-1} \frac{\partial \mathfrak{L}}{\partial (\mathcal{L}_n K_{ij})} = -\sqrt{h} \left[(\kappa^{-2} + \frac{\beta}{2} R) + 2\alpha C^{\text{minj}} \right], \quad (3.173b)$$

$$\Pi_{ij}^{(\lambda)} := \frac{\partial \underline{\mathfrak{L}}}{\partial \mathcal{L}_n \lambda^{ij}} = 0. \quad (3.173c)$$

At this stage note that the definition of \mathcal{P}^{ij} differs from Boulware's *choice*, which requires that \mathcal{P}^{ij} be zero at flat space. This option is adopted by Boulware because the linear term and the quadratic terms in the departing action are not treated on an equal footing in his formalism: The former is handled as in the ADM canonical version of general relativity whereas the latter are reduced to first order by means of a generalised Legendre transformation. In the formalism presented here—by contrast—we refrain to make such a segregation for we have shown previously that the generalised Ostrogradsky construction may be consistently applied to the ADM action (cf. Subsection 3.3.3).

The trace and traceless parts of \mathcal{P}^{ij} are respectively

$$\mathcal{P} = -3\sqrt{h}(\kappa^{-2} + \frac{\beta}{2}R), \quad \mathcal{P}^{\text{tij}} = -2\alpha\sqrt{h}C^{\text{minj}}. \quad (3.174)$$

The sole primary constraints of the general quadratic theory are $\varphi^{ij} \approx 0$ and $\Pi_{ij}^{(\lambda)} \approx 0$. Therefore, in agreement with the particle content of the theory, there are eight physical degrees of freedom.¹⁹

The next step in the Ostrogradsky construction consists in performing a generalised Legendre transformation. Here we want to solve the ‘velocities’ $\mathcal{L}_n K_{ij}$ for the canonical variables and their conjugate momenta. We achieve this goal by firstly solving equations (3.170) and (3.171b) for R and C^{minj} respectively, and then expressing these latter quantities in terms of \mathcal{P} and \mathcal{P}^{tij} respectively, with the help

¹⁹The number of physical degrees of freedom is determined by the equation $N_{\text{phys.}} = K - N_1 - \frac{1}{2}N_2$, where K is the total number of pairs of canonical variables, N_1 and N_2 are the number of first-class and second-class constraints respectively; see [HT92, p. 29].

of formulæ (3.174), thereby obtaining

$$\begin{aligned}\mathcal{L}_n K_{ij} = & -\frac{\mathcal{P}^{\text{T}ij}}{\alpha\sqrt{h}} + \frac{1}{3\beta}\left(\kappa^{-2} + \frac{\mathcal{P}}{3\sqrt{h}}\right)h_{ij} - \frac{N_{|ij}}{N} - {}^{(3)}R_{ij} \\ & - KK_{ij}\mathcal{P}^{ij} + \frac{\mathcal{P}}{2}({}^{(3)}R + K^2 - K_{ij}K^{ij}).\end{aligned}\quad (3.175)$$

Hence the restricted Hamiltonian density is

$$\begin{aligned}\mathfrak{H}_r(h, K, \mathcal{P}) = & \mathcal{P}^{ij}\mathcal{L}_n K_{ij} - N^{-1}\mathfrak{L} \\ = & \sqrt{h}(\alpha C_{\mathfrak{n}ijk}C^{\mathfrak{n}ijk} + V(\mathcal{P}) - \Lambda) + \frac{\mathcal{P}}{2}({}^{(3)}R + K^2 - K_{ij}K^{ij}) \\ & - \frac{\mathcal{P}^{\text{T}ij}\mathcal{P}_{ij}^{\text{T}}}{2\alpha\sqrt{h}} - \mathcal{P}^{ij}({}^{(3)}R_{ij} + KK_{ij} + N^{-1}N_{|ij}),\end{aligned}\quad (3.176)$$

where we have defined the ‘potential term’

$$V(\mathcal{P}) := \frac{1}{2\beta}\left(\kappa^{-2} + \frac{\mathcal{P}}{3\sqrt{h}}\right)^2. \quad (3.177)$$

The canonical Hamiltonian density is thus given by

$$\mathfrak{H}_c(h, K, p, \mathcal{P}) = \mathfrak{H}_r(h, K, \mathcal{P}) - 2p^{ij}K_{ij}. \quad (3.178)$$

Therefore, the Hamiltonian form of the gravitational action based on the original Lagrangian density (3.169) may be written as

$$\begin{aligned}S = \int dt \left[\int_{\Sigma_t} N \left(p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} - \mathfrak{H}_c(h, K, p, \mathcal{P}) \right) \right. \\ \left. - \oint_{S_t^\infty} \left(N \mathcal{P}^{jk}{}_{|j} - N_{|j} \mathcal{P}^{jk} \right) r_k \right],\end{aligned}\quad (3.179)$$

where the canonical Hamiltonian density is given by

$$\begin{aligned}\mathfrak{H}_c(h, K, p, \mathcal{P}) = & -2p^{ij}K_{ij} + \sqrt{h}(\alpha C_{\mathfrak{n}ijk}C^{\mathfrak{n}ijk} + V(\mathcal{P}) - \Lambda) \\ & - \frac{\mathcal{P}^{\text{T}ij}\mathcal{P}_{ij}^{\text{T}}}{2\alpha\sqrt{h}} + \frac{\mathcal{P}}{2}({}^{(3)}R + K^2 - K_{ij}K^{ij}) \\ & - \mathcal{P}^{ij}{}_{|ij} - \mathcal{P}^{ij}({}^{(3)}R_{ij} + KK_{ij}).\end{aligned}\quad (3.180)$$

Expanding the Lie derivatives in the action (3.179) and integrating by parts we obtain the final form of the quadratic canonical action, where we have retained all the surface terms, viz.

$$\begin{aligned}S = \int dt \left[\int_{\Sigma_t} N \left(p^{ij} \partial_t h_{ij} + \mathcal{P}^{ij} \partial_t K_{ij} - N\mathcal{H} - N^k \mathcal{H}_k \right) \right. \\ \left. - \oint_{S_t^\infty} \left[N \mathcal{P}^{jk}{}_{|j} - N_{|j} \mathcal{P}^{jk} + 2N_j (p^{jk} + \mathcal{P}^{ik} K^j{}_i) \right] r_k \right],\end{aligned}\quad (3.181)$$

where the super-Hamiltonian \mathcal{H} constraint coincides with the canonical Hamiltonian density (3.180) and the super-momentum constraint is given explicitly by

$$\mathcal{H}_k = \mathcal{P}^{ij} K_{ij|k} - 2(\mathcal{P}^{ij} K_{ik})_{|j} - 2h_{ik} p^{ij}_{|j}. \quad (3.182)$$

Remark. Since the constraints are local functions of the field quantities at a particular point of space, the Poisson bracket of two such objects is a sum of delta functions and derivatives of delta functions. In many instances it is simpler to integrate the constraints over the spatial sections with a test function: The constraint $\varphi(\mathbf{x}) \approx 0$ becomes

$$\varphi[\psi] := \int d^3x \psi(\mathbf{x}) \varphi(\mathbf{x}) \approx 0$$

and it must be functionally differentiated with respect to the canonical variables so that the Poisson bracket of two such (integrated) constraints be given by

$$\left\{ \varphi_A[\psi], \varphi_B[\psi'] \right\} := \int d^3x \left[\frac{\delta \varphi_A[\psi]}{\delta h_{kl}} \frac{\delta \varphi_B[\psi']}{\delta p^{kl}} + \frac{\delta \varphi_A[\psi]}{\delta K_{kl}} \frac{\delta \varphi_B[\psi']}{\delta \mathcal{P}^{kl}} - \left(\varphi_A \longleftrightarrow \varphi_B \right) \right], \quad (3.183)$$

where the canonical variables are varied freely, i.e. independently of the constraints.

The Poisson brackets involving the super-momentum constraint are easily calculated and understood, for \mathcal{H}_k is the generator of spatial diffeomorphisms. For instance, a direct application of the definition (3.183) yields

$$\left\{ G[\psi], h_{kl}(\mathbf{x}) \right\} = -\psi_{(k|l)}(\mathbf{x}),$$

where we have defined the integrated super-momentum as

$$G[\psi] := \int d^3x \mathcal{H}_m(\mathbf{x}) \psi^m(\mathbf{x}).$$

On the other hand, it is very difficult to compute the brackets involving the super-Hamiltonian constraint. (Such a tedious task was carried out by Boulware; see [Bou84, Appendix B].)

We now look at the possible simplifications that would arise if we specialised the generic quadratic action (3.169). Amongst the five distinct variants of the general theory, which were analysed by Buchbinder and Lyakhovich [BL87], only one turns out to be relevant for our purpose here, namely the conformally invariant theory ($\beta = 0$, $\Lambda = 0 = \kappa^{-1}$). Strictly speaking, the case $\alpha = 0$ —and in particular the pure R^2 theory—reduces to studying gravitational actions of the nonlinear type (cf. Subsection 3.3.2) whereas the cases corresponding to the vanishing of the sole coupling constant β may be set aside if one invokes the local conformal symmetry *ab initio*.

Conformally invariant theory. In the conformally invariant case the Lagrangian density is

$$\mathfrak{L} = -\alpha N \sqrt{h} \left(2C_{\mathfrak{m}ij} C^{\mathfrak{m}ij} + C_{\mathfrak{m}jk} C^{\mathfrak{m}jk} \right) \quad (3.184)$$

owing to the identity (3.172). The only alteration in the conjugate momenta (3.173) involves \mathcal{P}^{ij} , which becomes

$$\mathcal{P}^{ij} = -2\alpha \sqrt{h} C^{\mathfrak{m}ij}. \quad (3.185)$$

Now, in addition to $\varphi^{ij} \approx 0$ and $\Pi_{ij}^{(\lambda)} \approx 0$, we obtain the primary constraint

$$\phi = h_{ij} \mathcal{P}^{ij} = \mathcal{P} \approx 0, \quad (3.186)$$

which arises because only the traceless part of the ‘velocities’, i.e. $(\mathcal{L}_n K_{ij})^T$, can be extracted from equation (3.171b). Performing as usual a Legendre transformation on the appropriate extended Lagrangian density we obtain the canonical Hamiltonian density

$$\begin{aligned} \mathfrak{H}_c(h, K, p, \mathcal{P}) = & -2p^{ij} K_{ij} + \alpha \sqrt{h} C_{\mathfrak{m}jk} C^{\mathfrak{m}jk} - \frac{\mathcal{P}^{Tij} \mathcal{P}_{ij}^T}{2\alpha \sqrt{h}} \\ & - \mathcal{P}^{Tij}{}_{|ij} - \mathcal{P}^{Tij} ({}^{(3)}R_{ij} + K K_{ij}^T). \end{aligned} \quad (3.187)$$

Therefore, we may cast the conformally invariant action into canonical form, that is, up to boundary terms,

$$S = \int_{\mathcal{M}} N \left[p^{ij} \mathcal{L}_n h_{ij} + \mathcal{P}^{ij} \mathcal{L}_n K_{ij} - \mathfrak{H}_c(h, K, p, \mathcal{P}) \right]. \quad (3.188)$$

The associated Dirac Hamiltonian density is

$$\mathfrak{H}_{\mathcal{D}} = \mathfrak{H}_c + \mu_{kl} \varphi^{kl} + \nu^{kl} \Pi_{kl}^{(\lambda)} + \xi \phi. \quad (3.189)$$

Consistency of the primary constraints (3.186) when time evolution is considered yields the determination of the multipliers μ_{kl} and ν^{kl} and gives rise to the secondary constraint

$$\chi = 2p + K_{kl}^T \mathcal{P}^{Tkl} \approx 0. \quad (3.190)$$

According to the remark made on page 114, we may utilise test functions in order to simplify the computation of Poisson brackets. After tedious calculation we obtain

$$\left\{ G[\psi], \chi(\mathbf{x}) \right\} \propto (\psi^m \chi)_{|m}(\mathbf{x}) \approx 0, \quad \left\{ H[\zeta], \chi(\mathbf{x}) \right\} \propto \zeta(\mathbf{x}) \mathfrak{H}_c(\mathbf{x}) \approx 0,$$

where we have defined

$$H[\zeta] := \int d^3x \mathfrak{H}_c(\mathbf{x}) \zeta(\mathbf{x}).$$

Hence the constraint (3.190) is the unique secondary constraint stemming from the consistency algorithm. Furthermore it is first class—it is indeed the generator of conformal transformations—by virtue of the Poisson bracket

$$\left\{ \phi(\mathbf{x}), \chi(\mathbf{y}) \right\} = 2\mathcal{P} \delta(\mathbf{x} - \mathbf{y}) \approx 0.$$

Therefore, the number of physical degrees of freedom is six. This is in total agreement with the particle content of the linearised theory.

To proceed further we need to impose a gauge-fixing condition; we shall see in Chapter 4 how this can be realised, in the specific case of spatially homogeneous cosmologies, so that the trace of variables K_{ij} and \mathcal{P}^{ij} be removed from the set of canonical variables and the conformal constraint (3.190) be automatically satisfied.

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Chapter 4

Higher-order spatially homogeneous cosmologies

“This cosmos, which is the same for all, has not been made by any god or man, but it always has been, is, and will be, an ever-living fire, kindling itself by regular measures and going out by regular measures.”

— Heraclitus of Ephesus.

THE simplest class of space-times that give physically reasonable cosmological models are the famed Friedmann–Lemaître–Robertson–Walker (FLRW) spaces, which are isotropic and are homogeneous on spacelike sections. It is conventional wisdom that FLRW models describe faithfully the large-scale properties of our universe. They indeed successfully account for many of its observed features and constitute the basic pillar of the standard model of cosmology, which is not yet free from certain riddles: the so-called horizon, ‘flatness’, and ‘smoothness’ problems. These are addressed, more or less adequately, by incorporating the inflationary paradigm into the ‘bare old-fashioned’ isotropic cosmology and by invoking the existence of hot and cold dark matter blends. Be that as it may, mathematical cosmology cannot be satisfied with those models for their degree of simplicity, though it guarantees that one could easily find closed-form solutions, also implies that deeper investigations on specific issues—such as the asymptotic approach towards the initial singularity and the related question of the genericness of oscillatory, chaotic dynamical regimes—are screened by the stringent symmetry requirement that the universe be isotropic *ab initio*. Even though the observed universe seems to be highly isotropic, there may have been large anisotropies at an earlier epoch; in that respect, it is of great interest to understand why the actual

universe is so much less anisotropic than Einstein's field equations allow it to be in principle.

One possible answer is to consider, as Penrose surmises, that the 'initial conditions' logically entail a vanishing Weyl tensor to ensure an isotropic universe from its very inception; another attitude towards that problem, which we adopt below, proceeds through generalising the FLRW models by dropping the isotropy hypothesis while keeping spatial homogeneity.¹ In particular, this endows anisotropic cosmologies with a nonzero Weyl tensor, the existence of which may alter the character of the singularities that typically arise in cosmology (see, e.g., [CE79]). Moreover, the field equations remain ordinary differential equations since only time variations are nontrivial.

In Section 4.1 we give a short account of spatially homogeneous cosmologies: Firstly, we summarise the geometrical setting that enables one to define and classify the spatially homogeneous anisotropic Bianchi cosmological models (for a very good synthesis the reader is referred to [ESW97]); then we discuss briefly the specific problem of nonvanishing surface terms in the Lagrangian and Hamiltonian formulations of Bianchi cosmologies both in general relativity and higher-order theories of gravity.

In Section 4.2 we analyse the behaviour of the Bianchi-type IX model in the pure general quadratic theory of gravity on approach to the initial singularity in a four-dimensional space-time. This work was carried out in collaboration with S. Cotsakis, J. Demaret, and Y. De Rop [CDDQ93]. (We focus on the analytical treatment, leaving aside the details of the numerical analysis.) The—empty—Bianchi-type IX or *mixmaster* model is of fundamental importance in mathematical cosmology for it is the most general spatially homogeneous model and it contains the closed FLRW model as a special case. Its major feature is its—chaotic—oscillatory behaviour when one reaches the initial singularity. The question that is addressed in this respect is whether this behaviour is altered when one considers more general settings than general relativity such as, for instance, purely quadratic theories of gravity. In this framework we show that the mixmaster universe possesses a *non-chaotic* solution which is stable and we prove that the so-called BKL approximation scheme is structurally unstable.

In Section 4.3 we make use of the general Hamiltonian formalism that we have developed in Subsection 3.3.4 (p. 110 ff.) to study the specific case of spatially ho-

¹As isotropy at each point entails spatial homogeneity, anisotropic cosmologies constitute the first class of cosmological models that are (fairly) more general than the FLRW models; they have been extensively studied for a couple of decades. By contrast, it is only very recently that *inhomogeneous* cosmological models have regained a genuine interest amongst researchers; see Krasinski's 'encyclopædia' for a recent and thorough account [Kra97].

homogeneous cosmologies. Firstly, we adapt the Hamiltonian formalism to Misner's parameterisation; for this purpose we define a canonical transformation the virtue of which is to disentangle terms stemming respectively from the pure R -squared and Weyl-squared variants of the general quadratic theory. This is helpful since one is able to treat those cases separately, thereby simplifying the analysis. In the first variant (R -squared) we derive—for those Bianchi types admitting a canonical formulation—the super-Hamiltonian constraint, the *reduced* Hamiltonian density, and the corresponding canonical equations, which constitute an autonomous differential system; in particular, we solve the latter analytically for Bianchi type I and thereafter compare our results with those found in the literature; for the Bianchi-type IX model we reduce the (first-order) canonical equations to three coupled second-order differential equations for the physical degrees of freedom; finally, we extend the discussion to FLRW models. This work was first undertaken during my MSc [Que92] and was carried out with J. Demaret [DQ95]. In the second variant (Weyl-squared), referred to as *conformal gravity*, we consider the simplest spatially homogeneous space-time that exhibits nontrivial physical degrees of freedom, namely the Bianchi-type I model (the isotropic FLRW space-times are indeed conformally flat). We derive the explicit forms of the super-Hamiltonian and the constraint expressing the conformal invariance of the theory and we write down the system of canonical equations. To seek out exact solutions to this system we add extra constraints on the canonical variables and we go through a global involution algorithm which eventually leads to the closure of the constraint algebra. The Painlevé approach provides us with a proof of non-integrability, as a consequence of the presence of movable logarithms in the general solution of the problem.² We extract all possible particular solutions that may be written in closed analytical form. This enables one to demonstrate that the global involution algorithm has proven to be exhaustive in the search for exact solutions. Finally, we discuss the conformal relationship or absence thereof of our solutions with Einstein spaces. More specifically we show that the necessary condition for a Bianchi-type I space to be conformal to an Einstein space, obtained from purely geometrical considerations, becomes—in conformal gravity—a sufficient condition as well; this enables us to determine which solution amongst the whole set of exact solutions is *not* conformal to an Einstein space. This work was carried out in collaboration with J. Demaret and C. Scheen [DQS98] (see also [Que98]).

²I am indebted to C. Scheen for providing me with the material on the analytic structure of the Bianchi-type I model in conformal gravity (p. 169 ff.), which is partly contained in [DQS98]. For a thorough investigation on methods that probe the analytic structure of differential systems and their application to relativistic cosmology, the interested reader may consult Scheen's PhD thesis [Sch99].

4.1 Spatially homogeneous cosmologies

4.1.1 Geometrical setting

A four-dimensional space-time (\mathcal{M}, g_{ab}) is said to be *spatially homogeneous* if it possesses an r -dimensional isometry group $G^{(r)}$ (invariance group of the metric g_{ab}) that acts transitively on a one-parameter family of spacelike hypersurfaces, the orbits of the group³ (so that $r \geq 3$), which provides a natural slicing of the space-time. At any point q on any such hypersurface Σ there are (at least) three nonzero linearly independent Killing vector fields tangent to Σ . Since a Killing vector field ξ^a is completely determined by the values of ξ^a and $\nabla_a \xi_b$ at any point q of Σ , there can be at most $r_{\max} = \frac{1}{2}n(n+1)$ linearly independent Killing vector fields on a manifold of dimension n (see, e.g., [Wal84, Appendix C.3]); here, this means $3 \leq r \leq 6$. When $r = r_{\max}$, the Riemannian space has constant curvature. Furthermore, a theorem due to Fubini states that a Riemannian space (for $n > 2$) cannot admit an isometry group of dimension $r = \frac{1}{2}n(n+1) - 1$ (see, e.g., [Eis66]); here, this implies that the only possible values of r are 3, 4, and 6. If $r = 6$, the space-time is not only spatially homogeneous but also spatially isotropic, that is, locally spherically symmetric, and belongs to the FLRW class, which features maximally symmetric spacelike sections, i.e. sections of constant curvature.⁴ If $r = 4$, the space-time is locally rotationally symmetric (LRS); there exists a three-parameter subgroup $\overline{G}^{(3)}$ that acts either *simply* or *multiply* transitively on the spacelike hypersurfaces: The latter case includes the Kantowski–Sachs cosmological models (the orbits of the group are two-dimensional, maximally symmetric, and with positive constant curvature); the former corresponds to LRS Bianchi models and thus points to the last possible value of r , namely $r = 3$, which corresponds to the Bianchi class. Thus, if we set aside the Kantowski–Sachs models, we are left with isometry groups that act *simply* transitively on the spacelike hypersurfaces Σ , i.e. such that $\dim G = \dim \Sigma = 3$. Hence, in the light of the preceding discussion, we can state a more precise definition of Bianchi cosmologies: *A Bianchi cosmology is a model the metric of which admits a three-dimensional group of isometries that acts simply transitively on spacelike hypersurfaces Σ , which are surfaces of homogeneity in space-time.* The complete list of Bianchi cosmological models is obtained by classifying the three-parameter isometry groups, that is, the three-dimensional real Lie algebras generated by the associated Killing vector fields; the outcome is nine nonequivalent Bianchi types—or ten equivalence classes—, named

³The orbit of a point p under a group $G^{(r)}$ is the set of points into which p is moved by the action of all elements of the group.

⁴Note that in the case of space-times ($n = 4$), the ten-parameter Poincaré isometry group of flat space is an example of $G^{(10)}$; Minkowski and de Sitter space-times are maximally symmetric.

Table 4.1: The Bianchi types for class A.

a	n_1	n_2	n_3	Bianchi type	p	q
0	0	0	0	I	0	1
0	+1	0	0	II	3	2
0	0	+1	-1	VI ₀	5	3
0	0	+1	+1	VII ₀	5	3
0	+1	+1	-1	VIII	6	4
0	+1	+1	+1	IX	6	4

according to Bianchi's own terminology. Let us briefly sketch the classification procedure according to Wahlquist and Behr, Ellis and MacCallum, and Siklos.⁵

Suppose X_i for $i = 1, 2, 3$ form a basis of a three-dimensional Lie algebra with structure constants C^k_{ij} , which are defined through the commutators $[X_i, X_j] = C^k_{ij}X_k$ (they are antisymmetric and satisfy the Jacobi identity). Given C^k_{ij} , we can define a three-vector a^i and a symmetric 3×3 matrix n^{ij} by $a_i := \frac{1}{2}C^l_{li}$ and $n^{ij} := \epsilon^{ikl}(\frac{1}{2}C^j_{kl} - \delta^j_k a_l)$ respectively, where ϵ^{ijk} is the unique totally antisymmetric tensor satisfying $\epsilon^{ijk}\epsilon_{ijk} = 3! = 6$. It is easy to show that the structure constants can be written as $C^k_{ij} = n^{kl}\epsilon_{lij} + 2\delta^k_{[i}a_{j]}$. Substitution of this expression into the Jacobi identity yields the simple result $n^{ij}a_j = 0$. According to Ellis and MacCallum, the classification now gives two broad classes: 'class A' ($a_i = 0$) and 'class B' ($a_i \neq 0$); the resulting Lie algebras are divided into several types according to the rank and the (modulus of the) signature of n^{ij} . In class A there exist precisely six distinct Lie algebras whereas in class B there are only four possible values for the rank and the signature of n^{ij} . Some types (VI and VII) can be subclassified with the help of a further invariant h , which can be determined by the formula $a_i a_j = \frac{1}{2}h n^{kr} n^{ls} \epsilon_{rsi} \epsilon_{klj}$. The resulting algebraic classification is summarised in Table 4.1 and Table 4.2 (n_i for $i = 1, 2, 3$ denotes the diagonal elements of the symmetric matrix n^{ij} ; a is the nonzero component of the vector a_i obtained after a suitable rotation of axis and rescaling; the number p refers to the dimension of the orbits of the group—it is related to the automorphism degrees of freedom—; and the number q describes the degree of generality of the most general vacuum solution of each group type.) This completes the Bianchi classification.

Given the classification, one can seek for each Bianchi type the corresponding three-manifold endowed with a metric and isometry group of that type; this is

⁵For thorough reviews on the Bianchi–Behr classification and related questions see, e.g., [Mac73, Mac79a, Mac79b, Jan84, BS86].

Table 4.2: The Bianchi types for class B.

a	n_1	n_2	n_3	Bianchi type	p	q
1	0	0	0	V	3	1
1	0	0	+1	IV	5	3
1	0	+1	-1	III or VI ₋₁	5	3
$\sqrt{-h}$	0	+1	-1	VI _{h} ($h < 0$)	5	3
\sqrt{h}	0	+1	+1	VII _{h} ($h > 0$)	5	3

Table 4.3: Basis one-forms in Bianchi types I, II, V, and IX.

Type	I	II	V	IX
ω^i	dx	$dx - zdy$	dx	$\cos y \cos z dx - \sin z dy$
	dy	dy	$e^x dy$	$\cos y \sin z dx + \cos z dy$
	dz	dz	$e^x dz$	$-\sin y dx + dz$

achieved by choosing time and spatial congruences, and with the help of invariant one-forms (as well as the automorphism degrees of freedom in order to simplify the spatial metric [Sik80, Sik84, RE85]). We follow here the metric approach rather than the orthonormal frame approach (see [ESW97]). The spatially homogeneous metrics can be written as $ds^2 = -d\tau^2 + h_{ij}(\tau)\omega^i\omega^j$ or, in terms of an arbitrary time variable, as $ds^2 = -N^2(t)dt^2 + h_{ij}(t)\omega^i\omega^j$, where N is the lapse function and ω^i for $i = 1, 2, 3$ are the basis dual one-forms, which satisfy (owing to Cartan's first structure equations) the relation $d\omega^i = \frac{1}{2}C^i_{kj}\omega^j \wedge \omega^k$. The explicit formulæ for types I, II, V, and IX are summed up in Table 4.3.

4.1.2 Hamiltonian cosmology

Besides its interest with regard to quantisation, the Hamiltonian formulation of general relativity has also been applied to a large variety of cosmological problems—both classical and quantum. One can trace back this kind of investigation to DeWitt who specialised the canonical formalism to the closed FLRW model, which was viewed as a toy-model for quantum gravity [DeW67]. Independently, Misner laid the foundations of *Hamiltonian cosmology* [Mis69a, Mis69b], that is, the study of cosmological models by means of equations of motion in Hamiltonian form—to be more specific, through the ADM reduction procedure and with the introduction of the fruitful concept of *minisuperspace* [Mis72].

Typically, the advantage of the Hamiltonian treatment in general relativity is twofold. Firstly, it enables one to give an heuristic analysis of the generic asymptotic behaviour of Bianchi models near the singularity (and at late times) without doing lengthy calculations: The analysis is reduced to the qualitative description of the motion of a point in a plane under the influence of a time-dependent potential [Rya72, Ugg97]. This type of investigation constitutes the *qualitative Hamiltonian cosmology*. Secondly, the Hamiltonian formulation enables one to produce a Hamiltonian in a certain ‘Lagrangian canonical’ form that reveals the mathematical similarities amongst different ‘hypersurface-homogeneous’ models [UJR95].

As regards the scope of this thesis, such qualitative treatment of Bianchi dynamics is quite difficult to adopt for we are dealing with higher-order theories, having more degrees of freedom than general relativity; hence the aforementioned qualitative analysis by means of simple potential diagrams breaks down. Notwithstanding this hindrance we would like to examine whether the Hamiltonian methods might produce some simplification of the intricacies that occur when one deals with higher-order field equations. The first aspect we want to discuss has to do with the variational principle as applied to spatially homogeneous cosmological models and, more specifically, to Bianchi cosmologies.

Variational principle and boundary terms.

In Section 2.1 we have given a short account of the metric variational principle in general relativity, without any reference whatsoever to spatially homogeneous cosmologies. Now if one tries to derive the field equations of the various Bianchi types by means of the Hilbert variational principle, then in general (as was firstly noticed by Hawking [Haw69], then confirmed by MacCallum and Taub [MT72]) one will not obtain the correct field equations. It was firstly claimed—erroneously—that the origin of the trouble laid in the utilisation of non-coordinate frames to perform the calculations [Rya74].⁶ But the true reason was given by Sneddon [Sne76]: The requirement of spatial homogeneity prevents a boundary term being set equal to zero.⁷ However, it turns out that for class A Bianchi models this boundary term identically vanishes. More specifically, if the metric is assumed to be spatially homogeneous, then the spatial integration in the ADM form of the Einstein–Hilbert action (3.166) can be performed to give

$$S_{\text{ADM}} = \int dt \left[\pi_{\text{ADM}}^{ij} \partial_t h_{ij} - N \mathcal{H} - N^i \mathcal{H}_i - 2 \left(\pi_{\text{ADM}}^{ik} N_i - \frac{1}{2} \pi_{\text{ADM}} N^k \right) \Big|_k \right]. \quad (4.1)$$

⁶This is still advocated by Ryan [RW84].

⁷See also the remark on page 98.

On account of the formula given on page 6 the spatial divergence in the action (4.1) reduces to the expression

$$\left(\pi_{\text{ADM}}^{ik}N_i - \frac{1}{2}\pi_{\text{ADM}}N^k\right)_{|k} = \left(\pi_{\text{ADM}}^{ik}N_i - \frac{1}{2}\pi_{\text{ADM}}N^k\right)C_{jk}^j. \quad (4.2)$$

Hence, unless the trace of the structure coefficients vanishes—the condition $C_{jk}^j = 0$ is precisely the characterisation of class A Bianchi models—the variation of the ADM action with respect to the shift vector produces additional unwanted terms and results in a wrong super-momentum constraint. Although most class B models do not admit a Hamiltonian formulation, some particular nondiagonal and all diagonal⁸ models do: This can be achieved whenever the super-momentum constraint is holonomic, i.e. can be expressed as the vanishing of a total derivative; then it can be integrated and used to reduce the number of gravitational degrees of freedom [UJR95].

Since at the end of Chapter 3 we have developed a Hamiltonian formulation of the generic quadratic gravity theory it is natural to address the question of under which circumstances the spatial divergences occurring in the action vanish so as to warrant a well-posed variational principle. Consider the quadratic action (3.181) in canonical form and focus on the surface integral; assuming that the metric be spatially homogeneous and that spatial integration have been performed we readily identify the corresponding spatial divergence, namely

$$\left[N\mathcal{P}_{|j}^{jk} + 2N_j(p^{jk} + \mathcal{P}^{ik}K_i^j)\right]_{|k}. \quad (4.3)$$

From mere inspection it is obvious that the variation of this term will not vanish unless one considers class A models: the expression (4.3) is indeed proportional to the trace of the structure coefficients. Therefore, we end up with the same conclusion as in general relativity: All class A models do admit a Hamiltonian formulation. This result also holds for a nonlinear gravitational action, for the spatial divergence (4.3) becomes in that case

$$2\left[N_j(p^{jk} + \mathcal{P}K^{jk})\right]_{|k} \quad (4.4)$$

and is proportional to the trace of the structure coefficients as well.

Remark. Whereas the super-momentum constraint \mathcal{H}_k is automatically satisfied for all diagonal class A models in general relativity, this is not necessarily the case in higher-order gravity, for the expression (3.182) of \mathcal{H}_k is not as simple as in general relativity. As a matter of fact the first term in that expression is not

⁸For example, Sneddon has contrived a method to “heal” the variational principle in the specific case of the diagonal Bianchi-type V model [Sne76].

of the form $\mathfrak{A}^{ij}{}_{|j}$, where \mathfrak{A}^{ij} is a tensor density; a direct calculation shows it is zero for all diagonal class A Bianchi types but type VI_0 in the specific conformally invariant case.⁹ This means that, unless one considers the latter situation, one can always safely choose the shift vector to be zero, which is the usual assumption in Hamiltonian cosmology. By contrast, in the aforementioned peculiar case one must check that this very choice does not break the equivalence with the field equations.

4.2 The mixmaster universe in fourth-order gravity

4.2.1 On the mixmaster chaotic dynamics

The term ‘mixmaster’ refers to the Bianchi-type IX cosmological model in vacuum [Mis69a]; it suggests the nice features of the Bianchi-type IX dynamics, i.e. the oscillatory regimes on approach towards the initial singularity (see [LL89]). Recently, this terminology has also been used to discriminate amongst *asymptotically velocity dominated cosmological models* (where the spatial curvature terms in the Hamiltonian constraint become negligible as compared to the square of the expansion rate as the singularity is approached; this corresponds to a Kasner-like behaviour) and oscillatory-like cosmologies the prototype of which is Bianchi type IX (and type VIII), which is of fundamental importance with regard to the investigations that address the issue of the genericness of chaos in relativistic cosmology on approach towards the initial singularity and of the nature of that singularity when spatial homogeneity is relaxed—cf. the Belinskii–Khalatnikov–Lifshitz (BKL) conjecture—(see [Ber98], and references therein). Interest in the mixmaster dynamics has increased dramatically in the last fifteen years (see the review in [CLL98]); controversies have arisen on the chaotic nature of the Bianchi-type IX model and in particular on the problem of (diffeomorphism-)invariant characterisation of chaos in relativistic systems (see [HBC94]).

That the mixmaster dynamics be chaotic is now fairly well confirmed—though it has not yet reached the unambiguous status of a theorem—by means of different methodologies: qualitative methods, numerical techniques, and analytical tools. *Qualitative methods* embody: the BKL piecewise approximation methods [BKL70, KP72]; Hamiltonian methods (Misner, Ryan, and others) [Rya72, RS75, Ugg97]; and dynamical systems methods [WE97]. The BKL approach (see, e.g., [LL89]) has shown that the evolution in time of the mixmaster model can be approximated as a sequence of time periods (Kasner epochs and eras) during which certain terms in the field equations may be neglected, thereby leading to a description of the dynamics

⁹Making use of the variables defined on page 147 we indeed obtain $\mathcal{H}_1 \equiv 0 \equiv \mathcal{H}_2$ and $\mathcal{H}_3 = -\frac{2\sqrt{3}}{3}(\mathcal{P}_+K_- + \mathcal{P}_-K_+) \approx 0$ for type VI_0 .

in terms of the Bianchi-types I and II models, and ‘bounce laws’ from one Kasner era to the other that are sensitive to initial conditions [Bar82, CB83]. Hamiltonian cosmology (see Subsection 4.1.2) has reduced the analysis of the field equations to that of a time-dependent Hamiltonian system in two dimensions for a particle that bounces on moving ‘potential walls’, which approximate the time-dependent potentials characterising the various Bianchi types. The dynamical systems approach is based on the fact that Einstein’s field equations for spatially homogeneous cosmologies can be written as an autonomous system of first-order differential equations, thereby defining a dynamical system; it was initiated by Collins [CS71, Col71] and developed extensively by Bogoyavlensky [Bog85], Wainwright [WH89], and others. Historically, *numerical techniques* have proven to be misleading, but the associated controversies have been smoothed away. More reliable algorithms are now used, mainly to probe the structure of the singularity in inhomogeneous space-times [Ber98]. Most recently, Cornish and Levin gave a very strong indication pointing towards the chaotic character of the mixmaster model, by exploiting fractal methods [CL97a, CL97b].¹⁰ *Analytical tools* tackle the ‘chaoticity issue’ in terms of integrability concepts—integrability of differential systems, which is inherently encoded into their analytic structure. The Painlevé method (see p. 169 ff.), which provides such an analytical tool, rests on the *Painlevé property*—a differential system possesses this property if and only if its general solution is uniformisable or, equivalently, exhibits no movable critical singularities. Integrable systems are defined in the sense of Painlevé as those systems that possess the Painlevé property. The trivial part of the Painlevé method, known as the Painlevé test, produces *necessary* but not sufficient conditions for a system to enjoy the Painlevé property and requires local single-valuedness of the general solution in a vicinity of all possible families of movable singularities (see, e.g., [RGB89, Con94, Con99]). Notwithstanding the fact that it is not conclusive—especially for real-time chaos—the Painlevé method has proven to be helpful in understanding the intricate structure of systems such as the mixmaster model [LMC94]; even more, the fruitful interplay of the Painlevé method and complex-time numerical integrations has been exemplified very recently [SD97, Sch99].

It has also been demonstrated that the mixmaster chaotic behaviour, which appears in a four-dimensional space-time in general relativity, is generically sustained as one increases the space-time dimensionality up to ten, but disappears in any universe with space-time dimension greater than ten [DHS85, DHH⁺86, HJS87, EH87, DDH88]. So, in the context of general relativity, the mixmaster

¹⁰One must bear in mind, however, that the fractal structure is obtained numerically: One must still be cautious as regards the conclusions of that analysis, even if the whole construction is very interesting conceptually.

evolutionary picture is dimensionally dependent.

In the next subsection we address the question of whether this picture is sensibly modified when one considers more general frameworks—in particular, higher-order theories of gravity. One possible scope of this investigation would be to determine how general the features of chaotic evolution met in general relativity are in the framework of all possible physically interesting theories of gravity. This programme also hopes to shed new light into the cosmological structure of gravity theories with higher derivatives: One possibility would be, for instance, that nice nonchaotic properties emerge near the space-time singularity, as is the case for the mixmaster model in a theory described by a Lagrangian of the type $L = R + \gamma_1 R^2$ [BC89, Cot90] or by a scale-invariant Lagrangian such as $L = R^2$ [BS89, SZ93]. Here we examine the structure of the Bianchi-type IX cosmological model in the pure quadratic theory of gravity, i.e. the theory that is described by the action (2.16) without the Einstein–Hilbert term of general relativity.¹¹

4.2.2 Asymptotic analysis of the field equations

The vacuum field equations derived from the general quadratic action

$$S = \int_{\mathcal{M}} d^4x \left[\gamma_1 \mathfrak{L}_1 + \gamma_2 \mathfrak{L}_2 + \gamma_3 \mathfrak{L}_3 \right], \quad (4.5)$$

where γ_i for $i = 1, 2, 3$ denote coupling constants, are obtained by gathering the Euler–Lagrange derivatives (2.20) together, viz.

$$\begin{aligned} \gamma_1 \left(2\nabla^a \nabla^b R - 2g^{ab} \square R + \frac{1}{2} g^{ab} R^2 - 2R R^{ab} \right) + \gamma_2 \left(\frac{1}{2} g^{ab} R_{cd} R^{cd} + \nabla^a \nabla^b R \right. \\ \left. - 2R^{bcad} R_{cd} - \square R^{ab} - \frac{1}{2} g^{ab} \square R \right) + \gamma_3 \left(\frac{1}{2} R^{cdef} R_{cdef} g^{ab} - 2R^{cdeb} R_{cde}{}^a \right. \\ \left. - 4\square R^{ab} + 2\nabla^a \nabla^b R - 4R^{bcad} R_{cd} + 4R^{ca} R^b{}_c \right) = 0. \end{aligned} \quad (4.6)$$

We are interested in the behaviour of the spatially homogeneous Bianchi cosmological model of type IX, which is described by a metric of the form

$$ds^2 = -dt^2 + h_{ij}(t) \omega^i \omega^j, \quad (4.7)$$

where ω^i for $i = 1, 2, 3$ are the $\text{SO}(3)$ -invariant differential forms that characterise Bianchi type IX (given explicitly in Table 4.3). The induced three-metric is assumed to be diagonal and of the form

$$h_{ij} = \text{diag}[a^2(t), b^2(t), c^2(t)], \quad (4.8)$$

¹¹Discarding that term is consistent with our purpose since we consider asymptotic solutions to the field equations hereafter.

where a, b, c are the scale factors. Substituting the Bianchi-type IX metric (4.7) together with the explicit form (4.8) into the vacuum field equations (4.6) we obtain the mixmaster field equations in terms of the scale factors a, b , and c . We write only the mixed $(^0_0)$ - and $(^1_1)$ -components (the $(^2_2)$ - and $(^3_3)$ -components can be obtained from the $(^1_1)$ -component by cyclic permutations). The result is

$$[\gamma_1 \mathfrak{L}_1 + \gamma_2 \mathfrak{L}_2 + \gamma_3 \mathfrak{L}_3]_0^0 = 0, \quad (4.9a)$$

$$[\gamma_1 \mathfrak{L}_1 + \gamma_2 \mathfrak{L}_2 + \gamma_3 \mathfrak{L}_3]_1^1 = 0, \quad (4.9b)$$

where \mathfrak{L}_i^{ab} for $i = 1, 2, 3$ are the Euler-Lagrange derivatives associated with \mathfrak{L}_i for $i = 1, 2, 3$ respectively, which are written down extensively in the Appendix at the end of this section on page 142 ff. In equations (4.9) the contributions from R^2 , $R^{ab}R_{ab}$, and $R^{abcd}R_{abcd}$ can be easily identified since they are multiplied by γ_1 , γ_2 , and γ_3 respectively.

We now proceed to examine the evolution of the Bianchi IX model on approach to the singularity (occurring at $t = 0$); this is dictated by the system (4.9) supplemented by the remaining components of the field equations. The basic idea of the asymptotic method is based on the search for existence (or nonexistence) of chaotic behaviour in the Bianchi-type IX evolution according to the field equations (4.6), which is intimately connected to the nonexistence (or existence) of power-law asymptotic solutions of the system on approach to the singularity as $t \rightarrow 0$. This method was first applied successfully by Barrow and Cotsakis [BC89, Cot90] who showed that, in the nonlinear theory based on a Lagrangian $L = f(R)$ that is a polynomial function of the scalar curvature, the vacuum Bianchi-type IX model is nonchaotic and possesses monotonic, power-law asymptotes on approach to the singularity. Accordingly, we look for power-law asymptotes that, to lower order, have the form

$$(a, b, c) = (t^{p_1}, t^{p_2}, t^{p_3}) \quad (4.10)$$

as $t \rightarrow 0$. For simplicity we define constants q^s by

$$q^s = \sum_{i=1}^3 p_i^s. \quad (4.11)$$

Substituting the *ansatz* (4.10) into the Bianchi-type IX field equations (4.9a) and (4.9b) (similar terms appear in the $(^2_2)$ - and $(^3_3)$ -components) we obtain, for the $(^0_0)$ -component,

$$(\mathfrak{L}_1)_0^0 = \frac{1}{2}t^{-4}[q^2 + (q^1)^2 - 2q^1][3q^2 - (q^1)^2 + 6q^1] + [\star\star\star], \quad (4.12a)$$

$$(\mathfrak{L}_2)_0^0 = \frac{1}{2}t^{-4}[3(q^2)^2 - q^2(q^1)^2 + 2(q^1)^3 + 2q^2q^1 - 3q^2 - 3(q^1)^2] + [\star\star\star], \quad (4.12b)$$

$$(\mathfrak{L}_3)_0^0 = t^{-4}[3q^4 + 3(q^2)^2 - 4q^3q^1 + 4q^2q^1 - 6q^2] + [\star\star\star], \quad (4.12c)$$

and, for the $(^1_1)$ -component,

$$(\mathfrak{L}_1)_1^1 = \frac{1}{2}t^{-4}[4p_1(q^1 - 3) - q^2 - (q^1)^2 + 10q^1 - 24] \times [q^2 + (q^1)^2 - 2q^1] + [\star\star\star], \quad (4.13a)$$

$$(\mathfrak{L}_2)_1^1 = \frac{1}{2}t^{-4}[4p_1(q^1 - 3)(q^2 - 1) - (q^2)^2 - q^2(q^1)^2 + 2(q^1)^3 + 6q^2q^1 - 7q^2 - 11(q^1)^2 + 12q^1] + [\star\star\star], \quad (4.13b)$$

$$(\mathfrak{L}_3)_1^1 = \frac{1}{2}t^{-4}[8p_1(q^1 - 3)(p_1^2 - p_1q^1 + q^1 + q^2 - 2) - 2q^4 - 2(q^2)^2 + 8q^3 - 4q^2] + [\star\star\star], \quad (4.13c)$$

where the explicitly written terms correspond to Bianchi type I and $[\star\star\star]$ are additional terms generated by the Bianchi-type IX potential. We know that the only power-law solutions to the Bianchi-type I field equations derived from equations (4.6) in a four-dimensional space-time are [Der89, CDGM91]:

1. the well-known Kasner solution

$$ds^2 = -dt^2 + \sum_{i=1}^3 t^{2p_i} (dx^i)^2, \quad \text{with } q^1 = q^2 = 1, \quad (4.14)$$

where the p 's can be represented in the parametric form

$$p_1(s) = \frac{-s}{1+s+s^2}, \quad p_2(s) = \frac{s(1+s)}{1+s+s^2}, \quad p_3(s) = \frac{1+s}{1+s+s^2}, \quad (4.15)$$

where the *Kasner parameter* s varies in the range $s \geq 1$;

2. the isotropic solution

$$ds^2 = -dt^2 + \sum_{i=1}^3 t^{2p_i} (dx^i)^2, \quad \text{with } p_1 = p_2 = p_3 = \frac{1}{2}. \quad (4.16)$$

This plays a key rôle in determining the evolution of the Bianchi-type IX model near the singularity in the fourth-order theory of gravity described by the action (4.5): Looking for power asymptotes to the Bianchi type IX field equations amounts to looking for Kasner or isotropic asymptotes to these equations.

We consider the algebraic system $\{(4.12b), (4.12c), (4.13b), (4.13c)\}$. Firstly, we seek for Kasner asymptotic solutions of the form (4.10), (4.11), and (4.14). Most of the additional terms appearing in the equations are “nondangerous” in the sense that they grow slower than the t^{-4} contributions (present in the Bianchi-type I field equations): they are unimportant as we approach the singularity. However, the following terms, which appear in equations (4.13b) and (4.13c), namely

$$\begin{aligned} & \frac{15a^4}{8b^4c^4} - \frac{2a^2}{b^2c^2} \left(\frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} \right) + \frac{a^2}{b^2c^2} \left[\left(\frac{\dot{b}}{b} \right)^2 + \left(\frac{\dot{c}}{c} \right)^2 \right] \\ & - 2a\dot{a} \left(\frac{\dot{c}}{b^2c^3} + \frac{\dot{b}}{b^3c^2} \right) - \frac{2a^2\dot{b}\dot{c}}{b^3c^3} + \frac{\dot{a}^2}{b^2c^2} + \frac{2a\ddot{a}}{b^2c^2}, \end{aligned} \quad (4.17a)$$

and

$$\begin{aligned} & \frac{55a^4}{8b^4c^4} - \frac{7a^2}{b^2c^2} \left(\frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} \right) + \frac{8a^2}{b^2c^2} \left[\left(\frac{\dot{b}}{b} \right)^2 + \left(\frac{\dot{c}}{c} \right)^2 \right] \\ & - 12a\dot{a} \left(\frac{\dot{c}}{b^2c^3} + \frac{\dot{b}}{b^3c^2} \right) - \frac{a^2\dot{b}\dot{c}}{b^3c^3} + \frac{6\dot{a}^2}{b^2c^2} + \frac{12a\ddot{a}}{b^2c^2} \end{aligned} \quad (4.17b)$$

respectively, are of the form t^{-4+8p_1} (the very first terms in expressions (4.17a) and (4.17b)) and t^{-4+4p_1} (the remaining nine terms in expressions (4.17a) and (4.17b)). Since $p_1 < 0$ in the anisotropic case all these terms grow faster than t^{-4} as $t \rightarrow 0$: They will be the dominant ones in the field equations on approach to the singularity. Thus in this case “dangerous terms” appear in the Ricci-squared and Riemann-squared Euler-Lagrange expressions. This is completely analogous to what happens in general relativity as demonstrated by the BKL approximation method: At a certain stage the description of the asymptotic dynamics in terms of the Bianchi-type I Kasner solution breaks down and one must take into account the aforementioned “dangerous terms” in the field equations; the dynamics is then described by the Taub solution of the Bianchi-type II model and this corresponds to a transition from one “Kasner epoch” to another. Hence, in our case, one should retrieve the same kind of oscillatory behaviour as that found in general relativity by BKL on approach to the singularity as $t \rightarrow 0$. One can indeed explicitly check that the BKL solution [BKL70]

$$\begin{aligned} a^2 &= \frac{-2p_1\Lambda}{\cosh(2p_1\Lambda\tau)}, \\ b^2 &= b(0)^2 \exp[2\Lambda(p_1 + p_2)\tau] \cosh(2p_1\Lambda\tau), \\ c^2 &= c(0)^2 \exp[2\Lambda(p_1 + p_3)\tau] \cosh(2p_1\Lambda\tau), \end{aligned} \quad (4.18)$$

where $dt = abc d\tau$ and Λ is a constant, satisfies the field equations (4.9a) and (4.9b) for Bianchi type IX to leading order on approach to the singularity, wherein

only the “dangerous” and the “Kasnerian” terms—those containing four dots—have been retained.

On the other hand, if we introduce the asymptotic isotropic solution (4.16) in the algebraic system $\{(4.12b), (4.12c), (4.13b), (4.13c)\}$, it appears that all the terms in the equations are nondangerous. This proves the possibility of reaching the cosmological singularity in a monotonic, nonchaotic way.

The conclusion from this analysis is that the fourth-order Bianchi-type IX equations admit no anisotropic monotonic power-law solutions all the way to the singularity, but only an isotropic one, given by (4.16).

Now it is known that each vacuum solution of general relativity also satisfies the equations (4.6) in space-time dimension $n \leq 4$ since the R -squared equation (cf. (2.20a)) and the Ricci-squared equation (cf. (2.20b)) are obviously satisfied if $R_{ab} = R = 0$ and because the variation of the quadratic Lovelock Lagrangian identically vanishes in space-time dimension $n < 5$. However, the solution space of higher-order gravity is larger than in general relativity; in particular, the Kasner solution (4.14) is not the general solution of the Bianchi-type I model in the fourth-order theory based on the action (4.5). Therefore, it is natural to address the question of the stability of the exact polynomial solutions (4.14) and (4.16). This is achieved through a perturbation analysis.

Consider for instance the pure Riemann-squared theory and choose the parameterisation

$$T = \ln(t), \quad \alpha = \ln(a), \quad \beta = \ln(b), \quad \gamma = \ln(c). \quad (4.19)$$

The linearised field equations for small perturbations ϵ_1 , ϵ_2 , and ϵ_3 of $\alpha = p_1 T$, $\beta = p_2 T$, and $\gamma = p_3 T$ respectively are

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= x_3, \\ \dot{x}_3 &= \sum_{i=1}^9 f_i(p_1, p_2, p_3) x_i, \\ \dot{x}_4 &= x_5, \\ \dot{x}_5 &= x_6, \\ \dot{x}_6 &= \sum_{i=1}^3 f_{i+6}(p_2, p_3, p_1) x_i + \sum_{i=4}^9 f_{i-3}(p_2, p_3, p_1) x_i, \\ \dot{x}_7 &= x_8, \\ \dot{x}_8 &= x_9, \end{aligned} \quad (4.20)$$

$$\dot{x}_9 = \sum_{i=1}^6 f_{i+3}(p_3, p_1, p_2) x_i + \sum_{i=7}^9 f_{i-6}(p_3, p_1, p_2) x_i,$$

where we have defined

$$x_1 := \dot{\epsilon}_1, \quad x_4 := \dot{\epsilon}_2, \quad x_7 := \dot{\epsilon}_3,$$

and

$$\begin{aligned} f_1(p_1, p_2, p_3) &= (2p_1^2 - 2p_1p_2 - 2p_1p_3 + 3p_1 + p_2^2 + p_2 + p_3^2 + p_3 - 2) \\ &\quad \times (p_1 + p_2 + p_3 - 3), \\ f_2(p_1, p_2, p_3) &= -p_1(4p_2 + 4p_3 - 9) - p_2(2p_3 - 7) + p_1^2 + 7p_3 - 11, \\ f_3(p_1, p_2, p_3) &= -(2p_1 + 2p_2 + 2p_3 - 6), \\ f_4(p_1, p_2, p_3) &= [2p_2(p_3 - 2) + 3p_2^2 + p_3^2 + 2p_3 - 5]p_1 - p_1^2(p_2 + 2p_3 - 5) \\ &\quad - p_2(p_3^2 + 1) - 2p_2^3 + 3p_2^2, \\ f_5(p_1, p_2, p_3) &= p_1(2p_2 + 1) - p_1^2 - p_2^2 + p_2, \\ f_6(p_1, p_2, p_3) &= 0, \\ f_7(p_1, p_2, p_3) &= p_1[2p_2(p_3 + 1) + p_2^2 + 3p_3^2 - 4p_3 - 5] - p_1^2(2p_2 + p_3 - 5) \\ &\quad - p_2^2p_3 - 2p_3^3 + 3p_3^2 - p_3, \\ f_8(p_1, p_2, p_3) &= p_1(2p_3 + 1) - p_1^2 - p_3^2 + p_3, \\ f_9(p_1, p_2, p_3) &= 0. \end{aligned}$$

The characteristic polynomial related to the differential system (4.20) takes the forms

$$-(\lambda + 1)(\lambda - 2)^5(\lambda - 3)\lambda^2$$

for the Kasner solution (4.14) and

$$-\frac{1}{64}(2\lambda - 1)^2(2\lambda - 3)^3(2\lambda - 5)(\lambda + 1)(\lambda - 1)^2$$

for the isotropic solution (4.16). Hence the corresponding evolution laws for the perturbations are

$$\epsilon_i(T) \simeq c_{i0} + c_{i1} \exp(-T) + c_{i2}T + c_{i3} \exp(2T) + c_{i4} \exp(3T), \quad (4.21a)$$

$$\begin{aligned} \epsilon_i(T) &\simeq c'_{i0} + c'_{i1} \exp(-T) + c'_{i2} \exp(T/2) + c'_{i3} \exp(T) \\ &\quad + c'_{i4} \exp(3T/2) + c'_{i5} \exp(5T/2), \end{aligned} \quad (4.21b)$$

for $i = 1, 2, 3$, with the conditions

$$\begin{aligned}
c_{11} &= kp_1, & c_{21} &= kp_2, & c_{31} &= kp_3, \\
p_1 c_{12} + p_2 c_{22} + p_3 c_{32} &= 0, \\
c_{14} &= c_{24} = c_{34} = 0, \\
c'_{11} &= c'_{21} = c'_{31} = \frac{k}{2}, \\
c'_{12} + c'_{22} + c'_{32} &= 0, \\
c'_{13} + c'_{23} + c'_{33} &= 0, \\
c'_{15} &= c'_{25} = c'_{35} = 0,
\end{aligned}$$

where k is an arbitrary but—as it stems from the perturbation analysis—infiniteesimal constant. Both perturbations given in equations (4.21) grow exponentially for $T \rightarrow +\infty$: The corresponding solutions are unstable. The same conclusion seems to apply in the neighbourhood of the initial singularity, i.e. as $T \rightarrow -\infty$, due to the presence of the terms $c_{i1} \exp(-T)$, $c_{i2}T$ and $c'_{i1} \exp(-T)$. However, the mere rôle of the terms involving $\exp(-T)$ is to shift the position of the initial singularity on the time axis. More explicitly, looking at the scale factor α and assuming that $k \exp(-T) \ll 1$ we obtain

$$\begin{aligned}
\alpha(T) + \epsilon_1(T) &\simeq \alpha_0 + p_1 T + c_{11} \exp(-T) + c_{12} T \\
&\simeq \alpha_0 + p_1 \ln \left[\exp(T) (1 + k \exp(-T)) \right] + c_{12} T \\
&\simeq \alpha_0 + p_1 \ln(t + k) + c_{12} \ln(t)
\end{aligned} \tag{4.22a}$$

in the case of the Kasner metric and

$$\begin{aligned}
\alpha(T) + \epsilon_1(T) &\simeq \alpha_0 + \frac{1}{2} T + c'_{11} \exp(-T) \\
&\simeq \alpha_0 + \frac{1}{2} \ln \left[\exp(T) (1 + k \exp(-T)) \right] \\
&\simeq \alpha_0 + \frac{1}{2} \ln(t + k)
\end{aligned} \tag{4.22b}$$

for the isotropic solution. Similar relations hold for the scale factors β and γ .

In conclusion, due to the presence of the divergent logarithmic term in (4.22a) the Kasner metric (4.14) is unstable on approach to the singularity, but the isotropic metric (4.16) is stable. To resume, the important facts of our analysis are:

- The quadratic theory based on the action (4.5) admits no anisotropic polynomial solutions other than the Kasner solution (4.14). In general relativity this is the general—thus stable—solution to the Bianchi-type I model; this leads in the Bianchi-type IX case to a shift from a Kasner solution to another with a

different set of Kasner exponents, thereby giving rise to the characteristic oscillatory behaviour of the mixmaster universe. Here we have shown that the Kasner polynomial solution is itself an unstable solution of the Bianchi-type I fourth-order field equations. This implies that an oscillatory behaviour based on Kasner asymptotes cannot be generic in the Bianchi-type IX fourth-order dynamics. The typical mixmaster oscillatory behaviour is of zero measure amongst all possible behaviours since it is unstable with respect to small perturbations.¹²

- There exists one stable, isotropic and monotonic solution, given by the metric (4.16), which attracts sufficiently close trajectories in the phase space. Such a situation is not met in general relativity, for the isotropic metric (4.16) is not a solution of Einstein's vacuum field equations.

Inclusion of matter fields does not alter the conclusions since they become dynamically negligible near the singularity: In general relativity matter fields are negligible with respect to the dominant metric terms, which grow as t^{-2} as one approaches the singularity; in the fourth-order dynamics the metric terms grow typically as t^{-4} as $t \rightarrow 0$; hence matter terms do not influence the Bianchi-type IX evolution.

Remark. When the space-time dimension is greater than four, the Kasner metric is no more a Bianchi-type I solution to the fourth-order theory derived from the action (4.5) [CDGM91]. Therefore, it seems reasonable to conjecture that, in contrast to the general nondiagonal case of multidimensional spatially homogeneous cosmology in general relativity, it is impossible to build a mixmaster universe in the fourth-order Kaluza–Klein theory based on the BKL approximation scheme.

Appendix

We give here the mixed components of the Euler–Lagrange derivatives (2.20), specialised to Bianchi type IX.

$$\begin{aligned} \gamma_1(\mathfrak{L}_1)_0^0 = & -\gamma_1(4\ddot{a}\dot{a}a^{-2} + 4\ddot{a}\dot{b}a^{-1}b^{-1} + 4\ddot{a}\dot{c}a^{-1}c^{-1} - 2\dot{a}^2a^{-2} - 4\dot{a}\dot{a}^2a^{-3} - 4\ddot{a}\dot{b}a^{-1}b^{-1} \\ & + 4\ddot{a}\dot{b}^2a^{-1}b^{-2} + 8\ddot{a}\dot{b}\dot{c}a^{-1}b^{-1}c^{-1} - 4\ddot{a}\dot{c}a^{-1}c^{-1} - 4\dot{a}^3\dot{b}a^{-3}b^{-1} \\ & + 4\ddot{a}\dot{c}^2a^{-1}c^{-2} - 4\dot{a}^3\dot{c}a^{-3}c^{-1} + 4\dot{a}^2\ddot{b}a^{-2}b^{-1} - 6\dot{a}^2\dot{b}^2a^{-2}b^{-2} \\ & - 4\dot{a}^2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} + 4\dot{a}^2\ddot{c}a^{-2}c^{-1} - 6\dot{a}^2\dot{c}^2a^{-2}c^{-2} - 4\dot{a}^2a^{-4} \end{aligned}$$

¹²This is supported by the numerical analysis of the Bianchi-type IX field equations in fourth-order gravity [CDDQ93].

$$\begin{aligned}
& + 2\dot{a}^2 a^{-4} b^2 c^{-2} + 2\dot{a}^2 a^{-4} b^{-2} c^2 - 2\dot{a}^2 b^{-2} c^{-2} + 4\ddot{a} \ddot{b} a^{-1} b^{-1} \\
& + 8\ddot{a} \ddot{b} \dot{c} a^{-1} b^{-1} c^{-1} - 4\dot{a} \dot{b}^3 a^{-1} b^{-3} - 4\dot{a} \dot{b}^2 \dot{c} a^{-1} b^{-2} c^{-1} - 2\dot{a} \dot{b} a^{-1} b^{-3} \\
& + 8\dot{a} \dot{b} \dot{c} a^{-1} b^{-1} c^{-1} - 4\dot{a} \dot{b} \dot{c}^2 a^{-1} b^{-1} c^{-2} - \dot{a} \dot{b} a b^{-3} c^{-2} - \dot{a} \dot{b} a^{-3} b c^{-2} \\
& + 2\dot{a} \dot{b} a^{-1} b^{-1} c^{-2} - \dot{a} \dot{b} a^{-3} b c^{-2} - 2\dot{a} \dot{b} a^{-3} b^{-1} - 4\dot{a} \dot{c}^3 a^{-1} c^{-3} \\
& + 3\dot{a} \dot{b} a^{-3} b^{-3} c^2 + 4\ddot{a} \ddot{c} a^{-1} c^{-1} - \dot{a} \dot{c} a b^{-2} c^{-3} - \dot{a} \dot{c} a^{-3} b^{-2} c \\
& - 2\dot{a} \dot{c} a^{-1} c^{-3} + 2\dot{a} \dot{c} a^{-1} b^{-2} c^{-1} + 3\dot{a} \dot{c} a^{-3} b^2 c^{-3} - 2\dot{a} \dot{c} a^{-3} c^{-1} - 4\ddot{b} \dot{b}^2 b^{-3} \\
& + 4\ddot{b} \dot{b} \dot{b} b^{-2} + 4\ddot{b} \dot{c} b^{-1} c^{-1} - 2\dot{b}^2 b^{-2} + 4\dot{b} \dot{c}^2 b^{-1} c^{-2} - 4\dot{b} \dot{c} b^{-1} c^{-1} \\
& - 4\dot{b}^3 \dot{c} b^{-3} c^{-1} + 4\dot{b}^2 \dot{c} b^{-2} c^{-1} + 2\dot{b}^2 a^2 b^{-4} c^{-2} - 6\dot{b}^2 \dot{c}^2 b^{-2} c^{-2} \\
& + 2\dot{b}^2 a^{-2} b^{-4} c^2 - 2\dot{b}^2 a^{-2} c^{-2} - 4\dot{b} \dot{c}^3 b^{-1} c^{-3} - 4\dot{b}^2 b^{-4} + 4\ddot{b} \ddot{c} b^{-1} c^{-1} \\
& + 3\dot{b} \dot{c} a^2 b^{-3} c^{-3} - \dot{b} \dot{c} a^{-2} b c^{-3} - \dot{b} \dot{c} a^{-2} b^{-3} c + 2\dot{b} \dot{c} a^{-2} b^{-1} c^{-1} \\
& - \dot{b} \dot{c} a^{-2} b^{-3} c - 2\dot{b} \dot{c} b^{-1} c^{-3} - 2\dot{b} \dot{c} b^{-3} c^{-1} + 4\ddot{c} \dot{c} c^{-2} - 2\dot{c}^2 c^{-2} - 4\ddot{c} \dot{c}^2 c^{-3} \\
& + 2\dot{c}^2 a^2 b^{-2} c^{-4} + 2\dot{c}^2 a^{-2} b^2 c^{-4} - 2\dot{c}^2 a^{-2} b^{-2} - 4\dot{c}^2 c^{-4} + \frac{1}{8} a^4 b^{-4} c^{-4} \\
& - \frac{1}{2} a^2 b^{-2} c^{-4} - \frac{1}{2} a^2 b^{-4} c^{-2} - \frac{1}{2} a^{-2} b^2 c^{-4} + \frac{1}{2} a^{-2} b^{-2} - \frac{1}{2} a^{-2} b^{-4} c^2 \\
& + \frac{1}{2} a^{-2} c^{-2} + \frac{1}{8} a^{-4} b^4 c^{-4} - \frac{1}{2} a^{-4} b^2 c^{-2} - \frac{1}{2} a^{-4} b^{-2} c^2 + \frac{1}{8} a^{-4} b^{-4} c^4 \\
& + \frac{3}{4} a^{-4} + \frac{1}{2} b^{-2} c^{-2} + \frac{3}{4} b^{-4} + \frac{3}{4} c^{-4});
\end{aligned}$$

$$\begin{aligned}
\gamma_2(\mathfrak{L}_2)_0^0 = & -\gamma_2(2\ddot{a} \dot{a} a^{-2} + \ddot{a} \dot{b} a^{-1} b^{-1} + \ddot{a} \dot{c} a^{-1} c^{-1} - \ddot{a}^2 a^{-2} - 2\ddot{a} \dot{a}^2 a^{-3} + \ddot{a} \dot{a} \dot{b} a^{-2} b^{-1} \\
& + \ddot{a} \dot{a} \dot{c} a^{-2} c^{-1} - \ddot{a} \dot{b} a^{-1} b^{-1} + \ddot{a} \dot{b}^2 a^{-1} b^{-2} + 2\ddot{a} \dot{b} \dot{c} a^{-1} b^{-1} c^{-1} \\
& - \ddot{a} \dot{c} a^{-1} c^{-1} + \ddot{a} \dot{c}^2 a^{-1} c^{-2} - \dot{a}^3 \dot{b} a^{-3} b^{-1} + \dot{a}^2 \ddot{b} a^{-2} b^{-1} - \dot{a}^3 \dot{c} a^{-3} c^{-1} \\
& - 3\dot{a}^2 \dot{b}^2 a^{-2} b^{-2} - \dot{a}^2 \dot{b} \dot{c} a^{-2} b^{-1} c^{-1} - 3\dot{a}^2 \dot{c}^2 a^{-2} c^{-2} + \dot{a}^2 \dot{c} a^{-2} c^{-1} \\
& + \dot{a}^2 a^{-4} b^2 c^{-2} + \dot{a}^2 a^{-4} b^{-2} c^2 + \dot{a}^2 b^{-2} c^{-2} + \dot{a} \ddot{b} a^{-1} b^{-1} - 2\dot{a}^2 a^{-4} \\
& + \dot{a} \dot{b} \dot{b} a^{-1} b^{-2} - \dot{a} \dot{b}^3 a^{-1} b^{-3} - \dot{a} \dot{b}^2 \dot{c} a^{-1} b^{-2} c^{-1} + 2\dot{a} \dot{b} \dot{c} a^{-1} b^{-1} c^{-1} \\
& + 2\dot{a} \dot{b} \dot{c} a^{-1} b^{-1} c^{-1} - 2\dot{a} \dot{b} a b^{-3} c^{-2} - 2\dot{a} \dot{b} a^{-3} b c^{-2} - \dot{a} \dot{b} \dot{c}^2 a^{-1} b^{-1} c^{-2} \\
& + 2\dot{a} \dot{b} a^{-3} b^{-3} c^2 + \dot{a} \dot{c} \dot{c} a^{-1} c^{-2} - \dot{a} \dot{c}^3 a^{-1} c^{-3} + \dot{a} \ddot{c} a^{-1} c^{-1} \\
& - 2\dot{a} \dot{c} a b^{-2} c^{-3} - 2\dot{a} \dot{c} a^{-3} b^{-2} c + 2\ddot{b} \dot{b} \dot{b} b^{-2} + 2\dot{a} \dot{c} a^{-3} b^2 c^{-3} \\
& + \ddot{b} \dot{c} b^{-1} c^{-1} - 2\ddot{b} \dot{b}^2 b^{-3} + \ddot{b} \dot{c} b^{-2} c^{-1} - \ddot{b}^2 b^{-2} - \ddot{b} \dot{c} b^{-1} c^{-1} \\
& - \dot{b}^3 \dot{c} b^{-3} c^{-1} + \dot{b}^2 \dot{c} b^{-2} c^{-1} - 3\dot{b}^2 \dot{c}^2 b^{-2} c^{-2} + \dot{b} \dot{c}^2 b^{-1} c^{-2} + \dot{b}^2 a^{-2} b^{-4} c^2 \\
& + \dot{b}^2 a^2 b^{-4} c^{-2} + \dot{b}^2 a^{-2} c^{-2} - 2\dot{b}^2 b^{-4} - \dot{b} \dot{c}^3 b^{-1} c^{-3} + \dot{b} \dot{c} \dot{c} b^{-1} c^{-2} \\
& + \dot{b} \ddot{c} b^{-1} c^{-1} + 2\dot{b} \dot{c} a^2 b^{-3} c^{-3} + 2\ddot{c} \dot{c} c^{-2} - 2\dot{b} \dot{c} a^{-2} b c^{-3} - 2\dot{b} \dot{c} a^{-2} b^{-3} c \\
& - \dot{c}^2 c^{-2} + \dot{c}^2 a^2 b^{-2} c^{-4} + \dot{c}^2 a^{-2} b^2 c^{-4} + \dot{c}^2 a^{-2} b^{-2} - 2\ddot{c} \dot{c}^2 c^{-3} \\
& - 2\dot{c}^2 c^{-4} + \frac{3}{8} a^4 b^{-4} c^{-4} - \frac{1}{2} a^2 b^{-2} c^{-4} - \frac{1}{2} a^2 b^{-4} c^{-2} + \frac{1}{2} a^{-2} b^{-2} \\
& - \frac{1}{2} a^{-2} b^2 c^{-4} - \frac{1}{2} a^{-2} b^{-4} c^2 + \frac{1}{2} a^{-2} c^{-2} + \frac{3}{8} a^{-4} b^4 c^{-4} - \frac{1}{2} a^{-4} b^{-2} c^2
\end{aligned}$$

$$-\frac{1}{2}a^{-4}b^2c^{-2} + \frac{3}{8}a^{-4}b^{-4}c^4 + \frac{1}{4}a^{-4} + \frac{1}{2}b^{-2}c^{-2} + \frac{1}{4}b^{-4} + \frac{1}{4}c^{-4});$$

$$\begin{aligned} \gamma_3(\mathfrak{L}_3)_0^0 = & -\gamma_3(4\ddot{a}\dot{a}a^{-2} - 2\ddot{a}^2a^{-2} - 4\ddot{a}\dot{a}^2a^{-3} + 4\ddot{a}\dot{a}b^{-2}b^{-1} + 4\ddot{a}\dot{a}c^{-2}c^{-1} \\ & - 6\dot{a}^2\dot{b}^2a^{-2}b^{-2} - 6\dot{a}^2\dot{c}^2a^{-2}c^{-2} + 2\dot{a}^2a^{-4}b^2c^{-2} + 2\dot{a}^2a^{-4}b^{-2}c^2 \\ & + 6\dot{a}^2b^{-2}c^{-2} - 4\dot{a}^2a^{-4} + 4\dot{a}\ddot{b}b^{-1}b^{-2} - 7\dot{a}\dot{b}ab^{-3}c^{-2} \\ & + 2\dot{a}\dot{b}a^{-1}b^{-3} - 7\dot{a}\dot{b}a^{-3}bc^{-2} - 2\dot{a}\dot{b}a^{-1}b^{-1}c^{-2} + 2\dot{a}\dot{b}a^{-3}b^{-1} \\ & + 4\dot{a}\ddot{c}c^{-1}c^{-2} - 7\dot{a}\dot{c}ab^{-2}c^{-3} - 2\dot{a}\dot{c}a^{-1}b^{-2}c^{-1} + 5\dot{a}\dot{b}a^{-3}b^{-3}c^2 \\ & + 2\dot{a}\dot{c}a^{-1}c^{-3} + 5\dot{a}\dot{c}a^{-3}b^2c^{-3} - 7\dot{a}\dot{c}a^{-3}b^{-2}c + 2\dot{a}\dot{c}a^{-3}c^{-1} + 4\dot{b}\ddot{b}b^{-2} \\ & - 2\ddot{b}^2b^{-2} - 4\ddot{b}\dot{b}^2b^{-3} + 2\dot{b}^2a^2b^{-4}c^{-2} + 4\ddot{b}\dot{b}cb^{-2}c^{-1} - 6\dot{b}^2\dot{c}^2b^{-2}c^{-2} \\ & + 2\dot{b}^2a^{-2}b^{-4}c^2 + 6\dot{b}^2a^{-2}c^{-2} + 4\dot{b}\ddot{c}cb^{-1}c^{-2} + 5\dot{b}\dot{c}a^2b^{-3}c^{-3} - 4\dot{b}^2b^{-4} \\ & - 7\dot{b}\dot{c}a^{-2}bc^{-3} - 7\dot{b}\dot{c}a^{-2}b^{-3}c + 2\dot{b}\dot{c}b^{-1}c^{-3} - 2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} \\ & + 2\dot{b}\dot{c}b^{-3}c^{-1} - 2\dot{c}^2c^{-2} - 4\ddot{c}c^2c^{-3} + 2\dot{c}^2a^2b^{-2}c^{-4} + 4\dot{c}\ddot{c}c^{-2} \\ & + 2\dot{c}^2a^{-2}b^2c^{-4} + 6\dot{c}^2a^{-2}b^{-2} - 4\dot{c}^2c^{-4} + \frac{11}{8}a^4b^{-4}c^{-4} - \frac{3}{2}a^2b^{-4}c^{-2} \\ & - \frac{3}{2}a^2b^{-2}c^{-4} - \frac{3}{2}a^{-2}b^2c^{-4} + \frac{3}{2}a^{-2}b^{-2} - \frac{3}{2}a^{-2}b^{-4}c^2 + \frac{11}{8}a^{-4}b^4c^{-4} \\ & + \frac{3}{2}a^{-2}c^{-2} - \frac{3}{2}a^{-4}b^2c^{-2} - \frac{3}{2}a^{-4}b^{-2}c^2 + \frac{1}{4}a^{-4} + \frac{3}{2}b^{-2}c^{-2} \\ & + \frac{11}{8}a^{-4}b^{-4}c^4 + \frac{1}{4}b^{-4} + \frac{1}{4}c^{-4}); \end{aligned}$$

$$\begin{aligned} \gamma_1(\mathfrak{L}_1)_1^1 = & -\gamma_1(4\ddot{a}\dot{a}a^{-1} - 8\ddot{a}\dot{a}a^{-2} + 8\ddot{a}\dot{a}b^{-1}b^{-1} + 8\ddot{a}\dot{a}c^{-1}c^{-1} + 8\ddot{a}\dot{a}^2a^{-3} - 6\ddot{a}^2a^{-2} \\ & - 20\ddot{a}\dot{a}b^{-2}b^{-1} - 20\ddot{a}\dot{a}c^{-2}c^{-1} - 4\ddot{a}\dot{b}^2a^{-1}b^{-2} + 8\ddot{a}\dot{b}b^{-1}b^{-1} \\ & + 8\ddot{a}\dot{b}c^{-1}b^{-1}c^{-1} + 8\ddot{a}\dot{c}a^{-1}c^{-1} - 4\ddot{a}ab^{-2}c^{-2} - 4\ddot{a}\dot{c}^2a^{-1}c^{-2} \\ & + 4\ddot{a}a^{-3}b^2c^{-2} + 4\ddot{a}a^{-3}b^{-2}c^2 - 8\ddot{a}a^{-3} + 8\dot{a}^3\dot{c}a^{-3}c^{-1} + 8\dot{a}^3\dot{b}a^{-3}b^{-1} \\ & - 8\dot{a}^2\dot{b}a^{-2}b^{-1} + 2\dot{a}^2\dot{b}^2a^{-2}b^{-2} - 8\dot{a}^2\dot{c}a^{-2}c^{-1} - 12\dot{a}^2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} \\ & + 2\dot{a}^2\dot{c}^2a^{-2}c^{-2} - 6\dot{a}^2a^{-4}b^2c^{-2} + 4\dot{a}\ddot{b}b^{-1}b^{-1} - 6\dot{a}^2a^{-4}b^{-2}c^2 \\ & + 12\dot{a}^2a^{-4} - 2\dot{a}^2b^{-2}c^{-2} + 4\ddot{a}\dot{b}c^{-1}b^{-1}c^{-1} + 4\ddot{a}\dot{b}^3a^{-1}b^{-3} - 8\ddot{a}\dot{b}b^{-1}b^{-2} \\ & - 4\ddot{a}\dot{b}^2c^{-1}b^{-2}c^{-1} - 4\ddot{a}\dot{b}\dot{c}^2a^{-1}b^{-1}c^{-2} + 4\ddot{a}\dot{b}ab^{-3}c^{-2} + 4\ddot{a}\dot{b}\dot{c}a^{-1}b^{-1}c^{-1} \\ & + 12\ddot{a}\dot{b}a^{-3}bc^{-2} - 4\ddot{a}\dot{b}a^{-3}b^{-3}c^2 + 4\ddot{a}\dot{c}a^{-1}c^{-1} - 8\ddot{a}\dot{b}a^{-3}b^{-1} \\ & - 8\ddot{a}\dot{c}c^{-1}c^{-2} + 4\ddot{a}\dot{c}ab^{-2}c^{-3} - 4\ddot{a}\dot{c}a^{-3}b^2c^{-3} + 4\ddot{a}\dot{c}^3a^{-1}c^{-3} \\ & + 12\ddot{a}\dot{c}a^{-3}b^{-2}c + 4\ddot{b}\dot{b}b^{-1} - 4\ddot{b}\dot{b}b^{-2} + 8\ddot{b}\dot{c}b^{-1}c^{-1} - 8\ddot{a}\dot{c}a^{-3}c^{-1} \\ & - 2\ddot{b}^2b^{-2} - 8\ddot{b}\dot{b}cb^{-2}c^{-1} + 12\ddot{b}\dot{c}b^{-1}c^{-1} - 4\ddot{b}\dot{c}^2b^{-1}c^{-2} + 4\ddot{b}\dot{b}^2b^{-3} \\ & - \ddot{b}a^{-2}bc^{-2} - 2\ddot{b}a^{-2}b^{-1} + 3\ddot{b}a^{-2}b^{-3}c^2 + 2\ddot{b}b^{-1}c^{-2} - \ddot{b}a^2b^{-3}c^{-2} \\ & + 4\dot{b}^3\dot{c}b^{-3}c^{-1} - 4\dot{b}^2\dot{c}b^{-2}c^{-1} + 2\dot{b}^2\dot{c}^2b^{-2}c^{-2} - 4\dot{b}^2a^{-2}b^{-4}c^2 - 2\ddot{b}b^{-3} \end{aligned}$$

$$\begin{aligned}
& -4\dot{b}^2a^{-2}c^{-2} - 4\dot{b}^2a^2b^{-4}c^{-2} + 8\dot{b}^2b^{-4} + 8\dot{b}\ddot{c}b^{-1}c^{-1} + 4\dot{b}\dot{c}^3b^{-1}c^{-3} \\
& - 7\dot{b}\dot{c}a^2b^{-3}c^{-3} - 8\dot{b}\ddot{c}\dot{c}b^{-1}c^{-2} + 9\dot{b}\dot{c}a^{-2}bc^{-3} + 9\dot{b}\dot{c}a^{-2}b^{-3}c \\
& - 2\dot{b}\dot{c}b^{-1}c^{-3} - 2\dot{b}\dot{c}b^{-3}c^{-1} - 4\ddot{c}\dot{c}c^{-2} - 2\dot{c}^2c^{-2} - 2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} \\
& + 4\ddot{c}\dot{c}^2c^{-3} - \ddot{c}a^2b^{-2}c^{-3} - \ddot{c}a^{-2}b^{-2}c - 2\ddot{c}a^{-2}c^{-1} + 2\ddot{c}b^{-2}c^{-1} + 4\ddot{c}\ddot{c}c^{-1} \\
& + 3\ddot{c}a^{-2}b^2c^{-3} - 2\ddot{c}c^{-3} - 4\dot{c}^2a^{-2}b^{-2} + 8\dot{c}^2c^{-4} - 4\dot{c}^2a^{-2}b^2c^{-4} \\
& - 4\dot{c}^2a^2b^{-2}c^{-4} + \frac{5}{8}a^4b^{-4}c^{-4} - \frac{3}{2}a^2b^{-4}c^{-2} + \frac{1}{2}a^{-2}b^2c^{-4} - \frac{3}{2}a^2b^{-2}c^{-4} \\
& + \frac{1}{2}a^{-2}b^{-4}c^2 - \frac{1}{2}a^{-2}c^{-2} - \frac{3}{8}a^{-4}b^4c^{-4} + \frac{3}{2}a^{-4}b^2c^{-2} - \frac{1}{2}a^{-2}b^{-2} \\
& - \frac{3}{8}a^{-4}b^{-4}c^4 - \frac{9}{4}a^{-4} + \frac{3}{2}a^{-4}b^{-2}c^2 + \frac{1}{2}b^{-2}c^{-2} + \frac{3}{4}b^{-4} + \frac{3}{4}c^{-4});
\end{aligned}$$

$$\begin{aligned}
\gamma_2(\mathfrak{L}_2)_1 = & -\gamma_2(2\ddot{a}\ddot{a}a^{-1} - 4\ddot{a}\dot{a}a^{-2} + 4\ddot{a}\dot{b}a^{-1}b^{-1} + 4\ddot{a}\dot{c}a^{-1}c^{-1} - 3\dot{a}^2a^{-2} + 4\dot{a}\dot{a}^2a^{-3} \\
& - 7\dot{a}\dot{b}a^{-2}b^{-1} - 7\dot{a}\dot{c}a^{-2}c^{-1} + 3\dot{a}\dot{b}a^{-1}b^{-1} - 2\dot{a}\dot{b}^2a^{-1}b^{-2} \\
& + 4\dot{a}\dot{b}\dot{c}a^{-1}b^{-1}c^{-1} + 3\dot{a}\dot{c}a^{-1}c^{-1} - 2\dot{a}\dot{c}^2a^{-1}c^{-2} + 2\dot{a}\dot{a}b^{-2}c^{-2} \\
& + 2\dot{a}a^{-3}b^2c^{-2} + 2\dot{a}a^{-3}b^{-2}c^2 - 4\dot{a}a^{-3} + 2\dot{a}^3\dot{b}a^{-3}b^{-1} + 2\dot{a}^3\dot{c}a^{-3}c^{-1} \\
& - 2\dot{a}^2\dot{b}a^{-2}b^{-1} + \dot{a}^2\dot{b}^2a^{-2}b^{-2} - 3\dot{a}^2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} - 2\dot{a}^2\dot{c}a^{-2}c^{-1} \\
& + \dot{a}^2\dot{c}^2a^{-2}c^{-2} - 3\dot{a}^2a^{-4}b^2c^{-2} - 3\dot{a}^2a^{-4}b^{-2}c^2 + 6\dot{a}^2a^{-4} + \dot{a}^2b^{-2}c^{-2} \\
& + \dot{a}\ddot{b}a^{-1}b^{-1} - 4\dot{a}\ddot{b}b^{-1}b^{-2} + \dot{a}\ddot{b}\dot{c}a^{-1}b^{-1}c^{-1} + 2\dot{a}\dot{b}^3a^{-1}b^{-3} \\
& - 2\dot{a}\dot{b}^2\dot{c}a^{-1}b^{-2}c^{-1} + \dot{a}\dot{b}\dot{c}a^{-1}b^{-1}c^{-1} - 2\dot{a}\dot{b}\dot{c}^2a^{-1}b^{-1}c^{-2} - 2\dot{a}\dot{b}ab^{-3}c^{-2} \\
& + 6\dot{a}\dot{b}a^{-3}bc^{-2} - 4\dot{a}\dot{b}a^{-3}b^{-1} - 2\dot{a}\dot{b}a^{-3}b^{-3}c^2 + \dot{a}\ddot{c}a^{-1}c^{-1} \\
& - 4\dot{a}\ddot{c}a^{-1}c^{-2} + 2\dot{a}\dot{c}^3a^{-1}c^{-3} - 2\dot{a}\dot{c}ab^{-2}c^{-3} - 2\dot{a}\dot{c}a^{-3}b^2c^{-3} \\
& + 6\dot{a}\dot{c}a^{-3}b^{-2}c - 4\dot{a}\dot{c}a^{-3}c^{-1} + \ddot{b}b^{-1} - \ddot{b}\dot{b}b^{-2} + 2\ddot{b}\dot{c}b^{-1}c^{-1} \\
& + \ddot{b}\dot{b}^2b^{-3} - 2\ddot{b}\dot{b}\dot{c}b^{-2}c^{-1} + 3\ddot{b}\dot{c}b^{-1}c^{-1} - \ddot{b}\dot{c}^2b^{-1}c^{-2} - 2\ddot{b}a^2b^{-3}c^{-2} \\
& - 2\ddot{b}a^{-2}bc^{-2} + 2\ddot{b}a^{-2}b^{-3}c^2 + \dot{b}^3\dot{c}b^{-3}c^{-1} - \dot{b}^2\dot{c}b^{-2}c^{-1} + \dot{b}^2\dot{c}^2b^{-2}c^{-2} \\
& + \dot{b}^2a^2b^{-4}c^{-2} - 3\dot{b}^2a^{-2}b^{-4}c^2 - 3\dot{b}^2a^{-2}c^{-2} + 2\dot{b}^2b^{-4} + 2\dot{b}\ddot{c}b^{-1}c^{-1} \\
& - 2\dot{b}\ddot{c}\dot{c}b^{-1}c^{-2} + \dot{b}\dot{c}^3b^{-1}c^{-3} - 2\dot{b}\dot{c}a^2b^{-3}c^{-3} + 6\dot{b}\dot{c}a^{-2}bc^{-3} \\
& + 6\dot{b}\dot{c}a^{-2}b^{-3}c + \ddot{c}c^{-1} - \ddot{c}\dot{c}c^{-2} + \ddot{c}\dot{c}^2c^{-3} + 2\ddot{c}a^{-2}b^2c^{-3} - 2\ddot{c}a^2b^{-2}c^{-3} \\
& - 2\ddot{c}a^{-2}b^{-2}c + \dot{c}^2a^2b^{-2}c^{-4} - 3\dot{c}^2a^{-2}b^2c^{-4} + 2\dot{c}^2c^{-4} - 3\dot{c}^2a^{-2}b^{-2} \\
& + \frac{15}{8}a^4b^{-4}c^{-4} - \frac{3}{2}a^2b^{-2}c^{-4} - \frac{3}{2}a^2b^{-4}c^{-2} - \frac{1}{2}a^{-2}b^{-2} + \frac{1}{2}a^{-2}b^2c^{-4} \\
& + \frac{1}{2}a^{-2}b^{-4}c^2 - \frac{1}{2}a^{-2}c^{-2} - \frac{9}{8}a^{-4}b^4c^{-4} + \frac{3}{2}a^{-4}b^{-2}c^2 + \frac{3}{2}a^{-4}b^2c^{-2} \\
& - \frac{9}{8}a^{-4}b^{-4}c^4 - \frac{3}{4}a^{-4} + \frac{1}{2}b^{-2}c^{-2} + \frac{1}{4}c^{-4} + \frac{1}{4}b^{-4});
\end{aligned}$$

$$\begin{aligned}
\gamma_3(\mathfrak{L}_3)_1 = & -\gamma_3(4\ddot{a}\ddot{a}a^{-1} - 8\ddot{a}\dot{a}a^{-2} + 8\ddot{a}\dot{b}a^{-1}b^{-1} + 8\ddot{a}\dot{c}a^{-1}c^{-1} - 6\dot{a}^2a^{-2} + 8\dot{a}\dot{a}^2a^{-3}
\end{aligned}$$

$$\begin{aligned}
& -8\ddot{a}\dot{a}\dot{b}a^{-2}b^{-1} - 8\ddot{a}\dot{a}\dot{c}a^{-2}c^{-1} + 4\ddot{a}\ddot{b}a^{-1}b^{-1} - 4\ddot{a}\dot{b}^2a^{-1}b^{-2} \\
& + 8\ddot{a}\dot{b}\dot{c}a^{-1}b^{-1}c^{-1} + 4\ddot{a}\dot{c}a^{-1}c^{-1} - 4\ddot{a}\dot{c}^2a^{-1}c^{-2} + 12\ddot{a}ab^{-2}c^{-2} \\
& + 4\ddot{a}a^{-3}b^2c^{-2} + 4\ddot{a}a^{-3}b^{-2}c^2 - 8\ddot{a}a^{-3} + 2\dot{a}^2\dot{b}^2a^{-2}b^{-2} + 2\dot{a}^2\dot{c}^2a^{-2}c^{-2} \\
& - 6\dot{a}^2a^{-4}b^2c^{-2} - 6\dot{a}^2a^{-4}b^{-2}c^2 + 12\dot{a}^2a^{-4} + 6\dot{a}^2b^{-2}c^{-2} - 8\dot{a}\ddot{b}ba^{-1}b^{-2} \\
& + 4\dot{a}\dot{b}^3a^{-1}b^{-3} - 4\dot{a}\dot{b}^2\dot{c}a^{-1}b^{-2}c^{-1} - 4\dot{a}\dot{b}\dot{c}^2a^{-1}b^{-1}c^{-2} - 12\dot{a}\dot{b}ab^{-3}c^{-2} \\
& + 12\dot{a}\dot{b}a^{-3}bc^{-2} - 8\dot{a}\dot{b}a^{-3}b^{-1} - 4\dot{a}\dot{b}a^{-3}b^{-3}c^2 - 8\dot{a}\dot{c}\dot{c}a^{-1}c^{-2} \\
& + 4\dot{a}\dot{c}^3a^{-1}c^{-3} - 12\dot{a}\dot{c}ab^{-2}c^{-3} - 4\dot{a}\dot{c}a^{-3}b^2c^{-3} + 12\dot{a}\dot{c}a^{-3}b^{-2}c \\
& - 8\dot{a}\dot{c}a^{-3}c^{-1} + 2\dot{b}^2b^{-2} - 7\dot{b}a^2b^{-3}c^{-2} - 7\dot{b}a^{-2}bc^{-2} + 2\dot{b}a^{-2}b^{-1} \\
& + 5\dot{b}a^{-2}b^{-3}c^2 - 2\dot{b}b^{-1}c^{-2} + 2\dot{b}b^{-3} + 2\dot{b}^2\dot{c}^2b^{-2}c^{-2} + 8\dot{b}^2a^2b^{-4}c^{-2} \\
& - 8\dot{b}^2a^{-2}b^{-4}c^2 - 8\dot{b}^2a^{-2}c^{-2} - \dot{b}\dot{c}a^2b^{-3}c^{-3} + 15\dot{b}\dot{c}a^{-2}bc^{-3} \\
& + 2\dot{b}\dot{c}a^{-2}b^{-1}c^{-1} + 15\dot{b}\dot{c}a^{-2}b^{-3}c + 2\dot{b}\dot{c}b^{-1}c^{-3} + 2\dot{b}\dot{c}b^{-3}c^{-1} + 2\dot{c}^2c^{-2} \\
& - 7\dot{c}a^2b^{-2}c^{-3} + 5\dot{c}a^{-2}b^2c^{-3} - 7\dot{c}a^{-2}b^{-2}c + 2\dot{c}a^{-2}c^{-1} - 2\dot{c}b^{-2}c^{-1} \\
& + 2\dot{c}c^{-3} + 8\dot{c}^2a^2b^{-2}c^{-4} - 8\dot{c}^2a^{-2}b^2c^{-4} - 8\dot{c}^2a^{-2}b^{-2} + \frac{55}{8}a^4b^{-4}c^{-4} \\
& - \frac{9}{2}a^2b^{-2}c^{-4} - \frac{9}{2}a^2b^{-4}c^{-2} + \frac{3}{2}a^{-2}b^2c^{-4} - \frac{3}{2}a^{-2}b^{-2} + \frac{3}{2}a^{-2}b^{-4}c^2 \\
& - \frac{3}{2}a^{-2}c^{-2} - \frac{33}{8}a^{-4}b^4c^{-4} + \frac{9}{2}a^{-4}b^2c^{-2} + \frac{9}{2}a^{-4}b^{-2}c^2 - \frac{33}{8}a^{-4}b^{-4}c^4 \\
& - \frac{3}{4}a^{-4} + \frac{3}{2}b^{-2}c^{-2} + \frac{1}{4}b^{-4} + \frac{1}{4}c^{-4}).
\end{aligned}$$

4.3 Quadratic Hamiltonian cosmologies

4.3.1 Canonical formalism and Misner's parameterisation

We henceforth assume that the Bianchi-type metrics be diagonal so as to simplify the investigation.¹³ According to the possible forms of the Bianchi metrics, we start from the spatial element $dl^2 = h_{ij}(t)\omega^i\omega^j$ for which several parameterisations are equally acceptable; one usually adopts either $h_{ij} = \text{diag}[a^2(t), b^2(t), c^2(t)]$ or $h_{ij} = \text{diag}[e^{2\alpha(t)}, e^{2\beta(t)}, e^{2\gamma(t)}]$ as possible *ansatz*, with proper time or logarithmic time. It is useful to represent the anisotropic scale factors in terms of the logarithmic volume μ and orthogonal anisotropic ‘shears’ β_{\pm} . These prescriptions, first introduced by Misner, are simply¹⁴

$$\alpha = \mu + \beta_+ + \sqrt{3}\beta_-, \quad \beta = \mu + \beta_+ - \sqrt{3}\beta_-, \quad \gamma = \mu - 2\beta_+, \quad (4.23)$$

¹³This assumption might be wrong for some Bianchi types; the question of whether the Bianchi metrics are diagonalisable or not in generalised theories of gravity remains still unanswered.

¹⁴See, e.g., [Mis94].

and imply that the matrix formed with the β 's be traceless. Adopting Misner's parameterisation we may write the three-metrics of Bianchi models in the form

$$dl^2 = e^{2\mu} \left[e^{2(\beta_+ + \sqrt{3}\beta_-)} (\omega^1)^2 + e^{2(\beta_+ - \sqrt{3}\beta_-)} (\omega^2)^2 + e^{-4\beta_+} (\omega^3)^2 \right], \quad (4.24)$$

where μ , β_+ , and β_- are functions of time only and ω^i for $i = 1, 2, 3$ are the invariant differential forms that characterise the Bianchi type under study.

We rely on the Ostrogradsky canonical formalism of quadratic gravity theories developed in Subsection 3.3.4, which is completely generic, that is, applicable to space-times without isometries. Henceforth, we intend to specify this general Hamiltonian formalism to spatially homogeneous cosmologies. To this aim we perform an appropriate canonical transformation that renders Misner's parameterisation manifest: It maps the original set of Ostrogradsky canonical variables $\{h_{ij}, K_{ij}; p^{ij}, \mathcal{P}^{ij}\}$ onto the set¹⁵ $\{\mu, \beta_{\pm}, K_{\circ}, K_{\pm}; \Pi_{\mu}, \Pi_{\pm}, \mathcal{P}_{\circ}, \mathcal{P}_{\pm}\}$ and is explicitly defined according to the following prescriptions:

$$h_{11} = e^{2\mu} e^{2(\beta_+ + \sqrt{3}\beta_-)}, \quad h_{22} = e^{2\mu} e^{2(\beta_+ - \sqrt{3}\beta_-)}, \quad h_{33} = e^{2\mu} e^{-4\beta_+},$$

and

$$p^{ij} = \Pi^{ij} + K^{\text{T}i}_{\phantom{\text{T}i}k} \mathcal{P}^{\text{T}jk} + \frac{\mathcal{P}_{\circ}}{\sqrt{3}} K^{\text{T}ij} + \frac{K_{\circ}}{\sqrt{3}} \mathcal{P}^{\text{T}ij} + \frac{K_{\circ} \mathcal{P}_{\circ}}{3} h^{ij},$$

where the new momenta Π^{ij} are given by

$$\begin{aligned} \Pi^1_1 &= \frac{1}{12} (2\Pi_{\mu} + \Pi_+ + \sqrt{3}\Pi_-), \\ \Pi^2_2 &= \frac{1}{12} (2\Pi_{\mu} + \Pi_+ - \sqrt{3}\Pi_-), \\ \Pi^3_3 &= \frac{1}{6} (\Pi_{\mu} - \Pi_+), \end{aligned}$$

and the new K 's and \mathcal{P} 's by

$$\begin{aligned} K_{ij} &= K^{\text{T}}_{ij} + \frac{K_{\circ}}{\sqrt{3}} h_{ij}, & K^{\text{T}i}_{\phantom{\text{T}i}j} &= \frac{1}{\sqrt{6}} \text{diag}(K_+ + \sqrt{3}K_-, K_+ - \sqrt{3}K_-, -2K_+), \\ \mathcal{P}^{ij} &= \mathcal{P}^{\text{T}ij} + \frac{\mathcal{P}_{\circ}}{\sqrt{3}} h^{ij}, & \mathcal{P}^{\text{T}i}_{\phantom{\text{T}i}j} &= \frac{1}{\sqrt{6}} \text{diag}(\mathcal{P}_+ + \sqrt{3}\mathcal{P}_-, \mathcal{P}_+ - \sqrt{3}\mathcal{P}_-, -2\mathcal{P}_+). \end{aligned}$$

In terms of these new variables the original action in Hamiltonian form (3.179) becomes

$$S = \int dt \left[\Pi_{\mu} \dot{\mu} + \Pi_{\pm} \dot{\beta}_{\pm} + \mathcal{P}_{\circ} \dot{K}_{\circ} + \mathcal{P}_{\pm} \dot{K}_{\pm} - N\mathcal{H} - N_i \mathcal{H}^i \right], \quad (4.25)$$

¹⁵The symbol S_{\pm} stands for $\{S_+, S_-\}$ and the notation $A_{\pm}B_{\pm}$ must be understood as $A_+B_+ + A_-B_-$.

where the spatial integration $\int \omega^1 \wedge \omega^2 \wedge \omega^3$ has been performed. The super-Hamiltonian constraint is, in general, a quite complicated expression that is obtained by specifying the canonical Hamiltonian density (3.180) in terms of Bianchi isometries. For instance, the Bianchi-type IX super-Hamiltonian in the pure quadratic gravity theory is given explicitly by the expression¹⁶

$$\begin{aligned} \mathcal{H}_{\text{IX}} = & \alpha e^\mu \mathbf{C} \cdot \mathbf{C} - \mathbf{P} \cdot \mathbf{R} \\ & + \frac{\sqrt{6}}{3} \mathcal{P}_+ (K_-^2 - K_+^2) + \frac{\sqrt{3}}{3} K_\circ (K_\pm \mathcal{P}_\pm - \Pi_\mu) \\ & - \frac{\sqrt{6}}{6} K_\pm \Pi_\pm + \frac{2\sqrt{6}}{3} K_+ K_- \mathcal{P}_- + \frac{\sqrt{3}}{6} \mathcal{P}_\circ (K_+^2 + K_-^2) \\ & + \frac{2\sqrt{3}}{3} K_\circ^2 \mathcal{P}_\circ + \frac{1}{6\beta} e^{-3\mu} \mathcal{P}_\circ^2 - \frac{1}{2\alpha} e^{-3\mu} (\mathcal{P}_+^2 + \mathcal{P}_-^2), \end{aligned} \quad (4.26)$$

where we have denoted

$$\begin{aligned} \mathbf{C} \cdot \mathbf{C} := & e^{2\mu} C_{\text{ijk}} C^{\text{ijk}} \\ = & \frac{3}{2} K_+^2 \left[2e^{4\beta_+} (1 - \cosh(4\sqrt{3}\beta_-)) - 3e^{-8\beta_+} \right] \\ & + K_-^2 \left[4e^{-2\beta_+} \cosh(2\sqrt{3}\beta_-) - e^{4\beta_+} (1 + 7 \cosh(4\sqrt{3}\beta_-)) - \frac{1}{2} e^{-8\beta_+} \right] \\ & - 4\sqrt{3} K_+ K_- \left[e^{-2\beta_+} \sinh(2\sqrt{3}\beta_-) + e^{4\beta_+} \sinh(4\sqrt{3}\beta_-) \right] \end{aligned} \quad (4.27)$$

and

$$\begin{aligned} \mathbf{P} \cdot \mathbf{R} := & \mathcal{P}^{\text{Tij}} {}^{(3)}R_{ij} \\ = & e^{-2\mu} \left[\frac{\sqrt{6}}{3} \mathcal{P}_+ \frac{\partial \mathcal{V}}{\partial \beta_+} + \sqrt{2} \mathcal{P}_- \frac{\partial \mathcal{V}}{\partial \beta_-} + \frac{\sqrt{3}}{12} \mathcal{P}_\circ \mathcal{V}(\beta_+, \beta_-) \right], \end{aligned} \quad (4.28)$$

and where the function $\mathcal{V}(\beta_+, \beta_-)$ is given explicitly in Table 4.4 at the type IX entry.

As regards the super-momentum constraint, we reiterate that one may consistently choose the shift vector to be zero in all cases but type VI₀ (cf. the remark on page 132). To simplify the analysis we shall consider those canonical systems that correspond respectively to the pure R -squared and Weyl-squared variants of the general quadratic theory.

¹⁶The ensuing canonical equations are far more simpler to write down than the intricate Euler-Lagrange expressions given in the appendix of Section 4.2.

Table 4.4: Potentials for types I, II, VII₀, VIII, and IX.

Type	$\mathcal{V}(\beta_+, \beta_-)$
I	0
II	$\exp(-8\beta_+)$
VII ₀	$2 \exp(4\beta_+) [\cosh(4\sqrt{3}\beta_-) - 1]$
VIII	$\exp(-8\beta_+) + 2 \exp(4\beta_+) [\cosh(4\sqrt{3}\beta_-) - 1]$ $+ 4 \exp(-2\beta_+) \cosh(2\sqrt{3}\beta_-)$
IX	$\exp(-8\beta_+) + 2 \exp(4\beta_+) [\cosh(4\sqrt{3}\beta_-) - 1]$ $- 4 \exp(-2\beta_+) \cosh(2\sqrt{3}\beta_-)$

4.3.2 Pure R^2 Bianchi cosmologies

Reduced Hamiltonians and exact solutions

We first study the pure R -squared Bianchi cosmologies, the field equations of which were analysed by several authors with the aim of examining the asymptotic behaviour of the mixmaster model in that specific quadratic variant; see, e.g., [BS89, BC89, SZ93, Spi94]. In contradistinction to these works, we lay our analysis on the canonical system rather than the field equations. Our goal is to appraise the achievements of the Hamiltonian formalism; in particular, to determine whether it simplifies the investigation, and to compare our results with those that are published.

The canonical action (4.25) reduces to

$$S = \int dt \left[\Pi_\mu \dot{\mu} + \Pi_\pm \dot{\beta}_\pm + \mathcal{P}_\circ \dot{K}_\circ - N \mathcal{H} \right], \quad (4.29)$$

due to the existence of the primary constraint (3.139b), which translates into $\mathcal{P}_\pm \approx 0$ in terms of the new variables introduced in the preceding subsection. The super-Hamiltonian is

$$\begin{aligned} \mathcal{H} = & \frac{\sqrt{3}}{3} \left[2\mathcal{P}_\circ K_\circ^2 + \frac{1}{2}\mathcal{P}_\circ (K_+^2 + K_-^2) - K_\circ \Pi_\mu - \frac{\sqrt{2}}{2} K_\pm \Pi_\pm \right] \\ & + \frac{1}{6} e^{-3\mu} \mathcal{P}_\circ^2 - \frac{\sqrt{3}}{12} e^{-2\mu} \mathcal{P}_\circ \mathcal{V}(\beta_+, \beta_-), \end{aligned} \quad (4.30)$$

where $\mathcal{V}(\beta_+, \beta_-)$ denotes the potential of the Bianchi type considered (cf. Table 4.4), which stems from the three-dimensional scalar curvature, and the coupling constant β of the R -squared term in the action (3.169) has been set equal to one.

We must apply the Dirac–Bergmann consistency algorithm to this constrained system, the Poisson bracket being of course defined with respect to the new vari-

ables; or, equivalently, we can translate the results of Subsection 3.3.4 in terms of those variables. The Dirac Hamiltonian density is $\mathfrak{H}_{\mathcal{D}} = N\mathcal{H} + \lambda_{\pm}\mathcal{P}_{\pm}$, with Lagrange multipliers λ_{\pm} . Conservation of the primary constraints $\mathcal{P}_{\pm} \approx 0$ brings forth secondary constraints $\chi_{\pm} \approx 0$, viz.

$$\mathcal{P}_{\pm} \approx 0 \longrightarrow \chi_{\pm} = \mathcal{P}_{\circ}K_{\pm} - \frac{\sqrt{2}}{2}\Pi_{\pm} \approx 0,$$

the time evolution of which determines the Lagrange multipliers λ_{\pm} . Since we have the nonzero Poisson bracket $\{\mathcal{P}_{\pm}, \chi_{\pm}\} \approx -\mathcal{P}_{\circ}$ the above primary and secondary constraints are second class; hence the associated degrees of freedom, i.e. \mathcal{P}_{\pm} and K_{\pm} , are unphysical and can be removed. The super-Hamiltonian (4.30) becomes simply

$$\begin{aligned} \mathcal{H} = & \frac{\sqrt{3}}{3} \left[2\mathcal{P}_{\circ}K_{\circ}^2 - K_{\circ}\Pi_{\mu} - \frac{\Pi_{+}^2 + \Pi_{-}^2}{4\mathcal{P}_{\circ}} \right] + \frac{1}{6}e^{-3\mu}\mathcal{P}_{\circ}^2 \\ & - \frac{\sqrt{3}}{12}e^{-2\mu}\mathcal{P}_{\circ}\mathcal{V}(\beta_{+}, \beta_{-}), \end{aligned} \quad (4.31)$$

and the ensuing canonical equations are

$$\dot{\mu} = -\frac{\sqrt{3}}{3}NK_{\circ}, \quad (4.32a)$$

$$\dot{\beta}_{\pm} = -\frac{\sqrt{3}}{6}N\frac{\Pi_{\pm}}{\mathcal{P}_{\circ}}, \quad (4.32b)$$

$$\dot{K}_{\circ} = N \left[\frac{\sqrt{3}}{3} \left(2K_{\circ}^2 + \frac{\Pi_{+}^2 + \Pi_{-}^2}{4\mathcal{P}_{\circ}^2} \right) + \frac{1}{3}\mathcal{P}_{\circ}e^{-3\mu} - \frac{\sqrt{3}}{12}e^{-2\mu}\mathcal{V}(\beta_{+}, \beta_{-}) \right], \quad (4.32c)$$

$$\dot{\Pi}_{\mu} = N \left[\frac{1}{2}\mathcal{P}_{\circ}^2e^{-3\mu} - \frac{\sqrt{3}}{6}\mathcal{P}_{\circ}e^{-2\mu}\mathcal{V}(\beta_{+}, \beta_{-}) \right], \quad (4.32d)$$

$$\dot{\Pi}_{\pm} = \frac{3}{12}N\mathcal{P}_{\circ}e^{-2\mu}\frac{\partial\mathcal{V}}{\partial\beta_{\pm}}, \quad (4.32e)$$

$$\dot{\mathcal{P}}_{\circ} = -\frac{\sqrt{3}}{3}N(4K_{\circ}\mathcal{P}_{\circ} - \Pi_{\mu}). \quad (4.32f)$$

This canonical system possesses the first integral

$$\Pi_{\mu} - K_{\circ}\mathcal{P}_{\circ} = k_{\circ}, \quad (4.33)$$

where k_{\circ} is an arbitrary constant.

In the usual *minisuperspace* approaches of Hamiltonian cosmology one goes further by firstly fixing the lapse function, then solving the super-Hamiltonian for an adequately chosen canonical variable. The outcome is a *nonvanishing* ‘reduced’ Hamiltonian density. We proceed likewise and firstly consider space-times of non-constant scalar curvature.

Nonconstant scalar curvature. First of all, we fix the time gauge by setting

$$R = \rho e^t, \quad (4.34)$$

where $\rho = \pm 1$ (this allows for a separate discussion on space-times with positive or negative scalar curvature). According to the definition (3.174) the variable \mathcal{P}_\circ becomes

$$\mathcal{P}_\circ = -\frac{\sqrt{3}}{2}\rho e^{3\mu+t}. \quad (4.35)$$

Differentiating this expression and making use of the canonical equations (4.32) and the first integral (4.33) we obtain the form of the lapse function that corresponds to the gauge choice (4.34), namely

$$N(t) = \frac{\sqrt{3}}{k_\circ}\mathcal{P}_\circ = -\frac{3\rho}{2k_\circ}e^{3\mu+t}. \quad (4.36)$$

Solving the super-Hamiltonian (4.31) for K_\circ and performing the canonical transformation

$$\mu \longrightarrow \frac{1}{2}(\mu - t) \quad \Pi_\mu \longrightarrow 2\Pi_\mu + 3K_\circ\mathcal{P}_\circ$$

we obtain, after little algebraic manipulation, the reduced form of the Bianchi R -squared canonical action (4.29), namely

$$S = \int dt \left[\Pi_\mu \dot{\mu} + \Pi_\pm \dot{\beta}_\pm - H \right], \quad (4.37)$$

where the reduced Hamiltonian density is

$$H = \frac{1}{4k_\circ} \left[4\Pi_\mu^2 - \Pi_+^2 - \Pi_-^2 - \frac{3\rho^2}{4}e^{2\mu} \left(\rho e^\mu + \mathcal{V}(\beta_+, \beta_-) \right) + k_\circ^2 \right]. \quad (4.38)$$

The canonical equations are readily derived from the action (4.37), viz.

$$\dot{\mu} = \frac{2}{k_\circ}\Pi_\mu, \quad (4.39a)$$

$$\dot{\beta}_\pm = -\frac{1}{2k_\circ}\Pi_\pm, \quad (4.39b)$$

$$\dot{\Pi}_\mu = \frac{3\rho^2}{16k_\circ} [3\rho e^\mu + 2\mathcal{V}(\beta_+, \beta_-)] e^{2\mu}, \quad (4.39c)$$

$$\dot{\Pi}_\pm = \frac{3\rho^2}{16k_\circ} e^{2\mu} \frac{\partial \mathcal{V}}{\partial \beta_\pm}. \quad (4.39d)$$

They are equivalent to the autonomous system of second-order coupled ordinary differential equations

$$\ddot{\mu} = \frac{9\rho^3}{8k_o^2}e^{3\mu} + \frac{3\rho^2}{4k_o^2}e^{2\mu}\mathcal{V}(\beta_+, \beta_-), \quad (4.40a)$$

$$\ddot{\beta}_{\pm} = -\frac{3\rho^2}{32k_o^2}e^{2\mu}\frac{\partial\mathcal{V}}{\partial\beta_{\pm}}. \quad (4.40b)$$

By mere inspection, we see that the system (4.40) decouples when the potential term vanishes, i.e. for type I; hence we carry on to analysing the corresponding type I system.

From the canonical equation (4.39d) with zero potential, we conclude that the momenta Π_{\pm} are constants of motion. Hence we can readily integrate the equation (4.39b): the variables β_{\pm} are simply linear functions of t , namely

$$\beta_{\pm}(t) = -\frac{\Pi_{\pm}}{2k_o}t + b_{\pm}, \quad (4.41)$$

where the constants of integration b_{\pm} can be removed by a change of scale of the spatial coordinates. Furthermore, the equations (4.39a) and (4.39c) reduce to

$$\dot{\mu} = \frac{2}{k_o}\Pi_{\mu}, \quad (4.42a)$$

$$\dot{\Pi}_{\mu} = \frac{9\rho^3}{16k_o}e^{3\mu}. \quad (4.42b)$$

This is easy to solve and we obtain

$$e^{3\mu(t)} = \frac{64k_o^2\omega_o^2}{27\rho^3} \frac{n_o e^{2\omega_o t}}{(1 - n_o e^{2\omega_o t})^2}, \quad (4.43a)$$

$$\Pi_{\mu}(t) = \frac{k_o\omega_o}{3} \frac{1 + n_o e^{2\omega_o t}}{1 - n_o e^{2\omega_o t}}, \quad (4.43b)$$

where n_o is a new constant of integration and $\omega_o^2 := \frac{9}{4}[1 + (\Pi_+^2 + \Pi_-^2)/k_o^2]$. Therefore, the general Bianchi-type I metric is given by

$$ds^2 = -\frac{9\rho^2}{4k_o^2}e^{3\mu(t)}e^{-t}dt^2 + e^{\mu(t)}e^{-t}\sum_{i=1}^3 e^{2\nu_i t}(\mathrm{d}x^i)^2, \quad (4.44)$$

where the constants ν_i for $i = 1, 2, 3$ satisfy

$$\sum_{i=1}^3 \nu_i = 0, \quad \sum_{i=1}^3 \nu_i^2 = \frac{3}{2k_o^2}(\Pi_+^2 + \Pi_-^2) = \frac{2}{3}(\omega_o^2 - \frac{9}{4}).$$

Now, it is interesting to compare the form (4.44) of the general solution with those representations that were obtained by Buchdahl [Buc78] and independently

by Spindel and Zinque [SZ93] from a direct analysis of the Bianchi-type I higher-order field equations. In the former article the time coordinate is defined as $t_{[\text{B}]} = e^t$ and the logarithmic volume as $\mu_{[\text{B}]} = \frac{1}{2}(\mu - t)$ (with these relations one easily passes from the expression (4.44) to Buchdahl's solution); in the latter the time coordinate is given by $t_{[\text{SZ}]} = t$ whereas the variable $\Delta_{[\text{SZ}]}$ coincides with 3μ . Upon a mere redefinition of the constants of integration in the general solution (4.43a) we recover Spindel and Zinque's solution for $\Delta_{[\text{SZ}]}(t)$, namely

$$e^{\Delta_{[\text{SZ}]}(t)} = e^{3\mu(t)} = \frac{4}{3}Q^2a^2 \frac{e^{Qt}}{(1 - \rho\lambda^2a^2e^{Qt})^2}, \quad (4.45)$$

where Q^2 , λ^2 , and a^2 are positive constants defined in terms of ρ , k_\circ , ω_\circ , and n_\circ by

$$Q^2 := 4\omega_\circ^2, \quad \lambda^2 := \frac{9\rho^2}{4k_\circ^2}, \quad a^2 := \frac{4n_\circ k_\circ^2}{9\rho^3},$$

respectively. The proper time τ is obtained, up to constant factors, by integrating

$$\frac{d\tau}{dt} = \pm \frac{e^{\frac{1}{2}(Q-1)t}}{1 - \rho\lambda^2a^2e^{Qt}}. \quad (4.46)$$

We thus recover the two distinct behaviours of the general solution (4.45) found by Spindel and Zinque [SZ93] whose analysis of the Bianchi-type I field equations generalises Buchdahl's work [Buc78]. Strictly speaking, if $\rho = +1$, i.e. positive curvature, then the function in the right-hand side of equation (4.46) exhibits a vertical asymptote at $e^{Qt_\infty} = \lambda^{-2}a^{-2}$ corresponding to $\tau \rightarrow +\infty$; this behaviour features an asymptotic de Sitter space-time. On the other hand, if $\rho = -1$, i.e. negative curvature,¹⁷ then integration of equation (4.46) for $t \in \mathbb{R}$ yields a finite proper time after which the Bianchi-type I universe recollapses.

Remark. The metric (4.44) becomes isotropic if and only if $\Pi_\pm = 0$, i.e. $\omega_\circ = \frac{3}{2}$; that is, up to rescaled coordinates,

$$ds^2 = -\frac{e^{2t}}{(1 - n_\circ e^{3t})^2} dt^2 + \frac{dl^2}{(1 - n_\circ e^{3t})^{\frac{2}{3}}}. \quad (4.47)$$

Constant scalar curvature. When the scalar curvature is constant the field equations of the R -squared variant are satisfied by an arbitrary Einstein space, i.e. $R_{ab} = \frac{1}{4}Rg_{ab} = \Lambda g_{ab}$ with Λ constant. The problem of determining the general form of the metrics corresponding to Einstein spaces was undertaken by Petrov who proved, in particular, the following result [Pet69, p. 84].¹⁸

¹⁷This is the sole case considered by Buchdahl [Buc78].

¹⁸We have modified the original statement in accordance with our conventions and corrected a misprint.

Theorem 4.3.1. *The metric*

$$ds^2 = -(dx^n)^2 + \sum_{i=1}^{n-1} f_i(x^n) (dx^i)^2$$

defines a n -dimensional Einstein space $R_{ab} = \frac{1}{n} R g_{ab} = \Lambda g_{ab}$ if the functions f_i for $i = 1, \dots, n-1$ are chosen as follows:

$$f_i(x^n) = \begin{cases} \sin^{\frac{2}{n-1}}(\alpha x^n) \tan^{\frac{2\alpha_i}{\alpha}}(\frac{1}{2}\alpha x^n) & \text{if } \Lambda < 0, \\ \sinh^{\frac{2}{n-1}}(\beta x^n) \tanh^{\frac{2\beta_i}{\beta}}(\frac{1}{2}\beta x^n) & \text{if } \Lambda > 0, \end{cases} \quad (4.48)$$

where α , β , α_i , and β_i are constants; and if $\Lambda = 0$ one obtains either an S^n , i.e. a space of constant curvature, or the generalised Kasner metric¹⁹

$$f_i(x^n) = (x^n)^{2p_i}, \quad \text{with } \sum_{i=1}^{n-1} p_i = 1 = \sum_{i=1}^{n-1} p_i^2.$$

We demonstrate how the closed-form solution (4.48) can be derived from the canonical formalism, in the case $n = 4$ and for Bianchi type I.²⁰ First of all, observe that a constant scalar curvature, $R = 4\Lambda$, entails the vanishing of the constant k_o in the first integral (4.33) owing to the fact that the momentum \mathcal{P}_o reduces to $\mathcal{P}_o = -2\sqrt{3}\Lambda e^{3\mu}$; hence we have $\Pi_\mu = K_o \mathcal{P}_o$. We are free to fix a time gauge by choosing a specific lapse function. To recover Petrov's representation of Theorem 4.3.1 we could either start anew from the canonical equations (4.32) with zero potential and $N = 1$ or, equivalently, choose $N = \sqrt{3}\mathcal{P}_o$ and perform the transformation from the coordinate time t to the proper time τ on the result. In both cases we obtain the differential equation

$$\mathcal{P}_o'' - \omega_o^2 \mathcal{P}_o = 0, \quad (4.49)$$

where a prime denotes differentiation with respect to τ and $\omega_o^2 := 3\Lambda$. According to the sign of Λ there are two distinct solutions, which involve either trigonometric or hyperbolic functions, as this is expected from Theorem 4.3.1. For instance, if $\Lambda > 0$, then equation (4.49) integrates and gives $\mathcal{P}_o(\tau) = p_o \sinh(\omega_o \tau)$, where $p_o^2 = \frac{3}{4}(\Pi_+^2 + \Pi_-^2)/\omega_o^2$. The anisotropic shears are obtained upon integrating

$$\beta'_\pm + \frac{\sqrt{3}\Pi_\pm}{6p_o} \sinh^{-1}(\omega_o \tau) = 0; \quad (4.50)$$

¹⁹If $\Lambda = 0$ and $n = 4$, then the Kasner metric is the general solution.

²⁰The simple procedure given here yields the same results as Buchdahl's *modus operandi* [Buc78].

that is,

$$\beta_{\pm}(\tau) = -\frac{\sqrt{3}\Pi_{\pm}}{6\omega_{\circ}p_{\circ}} \ln \left| \tanh\left(\frac{\omega_{\circ}\tau}{2}\right) \right|. \quad (4.51)$$

Therefore, the general form of the metric can be written, up to rescaled constant factors, as

$$ds^2 = -d\tau^2 + \sinh^{\frac{2}{3}}(\omega_{\circ}\tau) \sum_{i=1}^3 \left[\tanh\left(\frac{\omega_{\circ}\tau}{2}\right) \right]^{\frac{2\nu_i}{\omega_{\circ}}} (dx^i)^2, \quad (4.52)$$

where the parameters ν_i satisfy the identities

$$\sum_{i=1}^3 \nu_i = 0, \quad \sum_{i=1}^3 \nu_i^2 = \frac{2}{3}\omega_{\circ}^2 = 2\Lambda.$$

We have thus recovered Petrov's representation (4.48) for the positive-curvature case.²¹

Remark. As this was first noticed by Buchdahl for a negative scalar curvature [Buc78], if one defines the new parameters $\tau^* := \frac{2}{\omega_{\circ}} \tanh(\frac{1}{2}\omega_{\circ}\tau)$ and $p_i := \nu_i/\omega_{\circ} + \frac{1}{3}$ for $i = 1, 2, 3$, then one may take the limit of the spatial element in the metric (4.52) as Λ tends to zero:

$$\lim_{\omega_{\circ} \rightarrow 0} \left[\cosh^{\frac{2}{3}}(\omega_{\circ}\tau) \sum_{i=1}^3 (\tau^*)^{2p_i} (dx^i)^2 \right] = \sum_{i=1}^3 \tau^{2p_i} (dx^i)^2,$$

where the parameters p_i satisfy the relations

$$\sum_{i=1}^3 p_i = 1, \quad \sum_{i=1}^3 p_i^2 = 1.$$

This is precisely the Kasner metric.

Isotropic models

Consider the closed FLRW cosmological model, which is contained in Bianchi type IX, the three-metric of which is

$$dl^2 = A^2(t) \left[\frac{dr^2}{1-r^2} + r^2 d\Omega^2 \right], \quad (4.53)$$

²¹One may proceed likewise for $\Lambda < 0$: the hyperbolic functions in the solution (4.52) are then replaced by the corresponding trigonometric ones (cf. [Buc78]).

where $d\Omega^2 = d\vartheta^2 + \sin^2(\vartheta)d\varphi$; r , ϑ , φ are the spherical coordinates; and $A(t)$ is the scale factor.

We take A and $K_\circ := \frac{\sqrt{3}}{3}A^2K$ as configuration variables; their respective conjugate momenta are $\Pi_A := 6Ap^{ij}$ (for $i = j$) and $\mathcal{P}_\circ := \frac{\sqrt{3}}{3}A^{-2}\mathcal{P}$. For an arbitrary nonlinear Lagrangian the latter momentum becomes $\mathcal{P}_\circ := -2\sqrt{3}Af'(R)$ according to the definition (3.138b). The canonical action is simply

$$S = \int dt [\Pi_A \dot{A} + \mathcal{P}_\circ \dot{K}_\circ - N\mathcal{H}], \quad (4.54)$$

where the super-Hamiltonian is

$$\mathcal{H} = \sqrt{3}\mathcal{P}_\circ - \frac{\sqrt{3}}{3}K_\circ \frac{\Pi_A}{A} + V(\mathcal{P}_\circ), \quad (4.55)$$

with the potential V defined by the expression (3.143).

For instance, if one considers the Einstein–Hilbert Lagrangian with an additional R -squared term (cf. the Lagrangian density (3.169) with $\Lambda = 0 = \alpha$), then the above potential reduces to $V(\mathcal{P}_\circ) = \frac{1}{2\beta}A(\frac{\sqrt{3}}{3}\mathcal{P}_\circ + \kappa^{-2}A)^2$. The quantum cosmology based on such a variant of the generic quadratic theory was investigated by Hawking and Luttrell [HL84]. They showed that the wave function of the closed FLRW minisuperspace universe could be interpreted as corresponding in the classical limit to a family of—particular—solutions that feature a period of inflation followed by a matter-dominated era. This era exhibits a rapidly oscillating scale factor superimposed on an overall expansion, after which the universe recollapses. A direct comparison with Hawking and Luttrell’s canonical formalism shows that their canonical Hamiltonian coincides exactly with the super-Hamiltonian (4.55) (with the specific aforementioned potential) if the lapse function is taken as $N(t) := A(t)$ and once the trivial canonical transformation $\{Q_{[\text{HL}]} \rightarrow \mathcal{P}_\circ; \Pi_{Q_{[\text{HL}]}} \rightarrow -K_\circ\}$ from their variables to ours has been performed.

We henceforth investigate the pure R -squared variant of the generic nonlinear case. The super-Hamiltonian is given by

$$\mathcal{H} = \sqrt{3}\mathcal{P}_\circ - \frac{\sqrt{3}}{3}K_\circ \frac{\Pi_A}{A} + \frac{1}{6}A\mathcal{P}_\circ^2 \quad (4.56)$$

and the ensuing canonical system,

$$\dot{A} = -\frac{\sqrt{3}}{3}N\frac{K_\circ}{A}, \quad (4.57a)$$

$$\dot{K}_\circ = N\left(\frac{1}{3}A\mathcal{P}_\circ + \sqrt{3}\right), \quad (4.57b)$$

$$\dot{\Pi}_A = -N\left(\frac{1}{6}\mathcal{P}_\circ^2 + \frac{\sqrt{3}}{3}K_\circ\frac{\Pi_A}{A^2}\right), \quad (4.57c)$$

$$\dot{\mathcal{P}}_\circ = \frac{\sqrt{3}}{3}N\frac{\Pi_A}{A}, \quad (4.57d)$$

possesses the first integral

$$A\Pi_A + K_{\circ}\mathcal{P}_{\circ} = k_{\circ}, \quad (4.58)$$

where k_{\circ} is an arbitrary constant. Firstly, we consider space-times of nonconstant scalar curvature.

Nonconstant scalar curvature. First of all, we fix the time gauge by setting

$$R = \rho e^t, \quad (4.59)$$

where $\rho = \pm 1$. According to its definition the variable \mathcal{P}_{\circ} becomes

$$\mathcal{P}_{\circ} = -\frac{\sqrt{3}}{2}\rho A e^t. \quad (4.60)$$

Differentiating this expression and making use of the canonical equations (4.57) and the first integral (4.58) we obtain the form of the lapse function that corresponds to the gauge choice (4.59), namely

$$N(t) = -\frac{3\rho}{2k_{\circ}}A^3 e^t. \quad (4.61)$$

Solving the super-Hamiltonian (4.56) for K_{\circ} and performing the canonical transformation

$$A \longrightarrow e^{\frac{1}{2}(\alpha-t)} \quad \Pi_A \longrightarrow 2\left(\Pi_{\alpha} + \frac{k_{\circ}}{2}\right)e^{-\frac{1}{2}(\alpha-t)}$$

we obtain the reduced form of the departing canonical action, namely

$$S = \int dt [\Pi_{\alpha}\dot{\alpha} - H], \quad (4.62)$$

where the reduced Hamiltonian density is

$$H = \frac{1}{4k_{\circ}}\left[4\Pi_{\alpha}^2 - \frac{3\rho^3}{4}e^{3\alpha} + 9\rho^2 e^{2\alpha} + k_{\circ}^2\right]. \quad (4.63)$$

The resulting canonical system,

$$\dot{\alpha} = \frac{2}{k_{\circ}}\Pi_{\alpha}, \quad (4.64a)$$

$$\dot{\Pi}_{\alpha} = \frac{9\rho^3}{16k_{\circ}}e^{3\alpha} - \frac{9\rho^2}{2k_{\circ}}e^{2\alpha}, \quad (4.64b)$$

is equivalent to the autonomous second-order differential equation²²

$$\ddot{\alpha} = \frac{9\rho^3}{8k_{\circ}^2}e^{3\alpha} - \frac{9\rho^2}{k_{\circ}^2}e^{2\alpha}, \quad (4.65)$$

²²Observe that this equation is nothing else than equation (4.40a) particularised to the isotropic case.

which can be formally solved: its general solution is given in terms of elliptic integrals.²³

Constant scalar curvature. When the scalar curvature is constant, i.e. $R = 4\Lambda$, we obtain from the canonical system (4.57) (with $N = 1$) the elementary second-order ordinary differential equation

$$\ddot{A} - \omega^2 A = 0, \quad (4.66)$$

where we have defined $\omega^2 := \frac{\Lambda}{3}$, and the first integral

$$\dot{A}^2 - \omega^2 A^2 + 1 = 0. \quad (4.67)$$

Once again there are two distinct cases depending on whether the scalar curvature be positive or negative:

$$A(t) = \begin{cases} \Lambda^{-\frac{1}{2}} \cosh(\sqrt{\Lambda}t) & \text{if } \Lambda > 0, \\ |\Lambda|^{-\frac{1}{2}} \cos(\sqrt{|\Lambda|}t) & \text{if } \Lambda < 0, \end{cases} \quad (4.68)$$

where we have rescaled the coordinates to eliminate irrelevant numerical factors. The former corresponds asymptotically to the de Sitter space-time.

Remark. When the scalar curvature is zero, the general solution to the canonical system (4.57) (with $N = 1$) is readily found; it is explicitly $A(t) = \sqrt{c_1 + c_2 t - t^2}$, where c_1 and c_2 are constants of integration, and contains the special solution that corresponds to an Einstein space filled with incoherent radiation (cf. [Sch93]).

Einstein-de Sitter minisuperspace. The three-metric of the Einstein-de Sitter model is

$$dl^2 = A^2(t)(dx^2 + dy^2 + dz^2). \quad (4.69)$$

We proceed as in the case of the closed FLRW model. The super-Hamiltonian is

$$\mathcal{H} = \frac{1}{6}A\mathcal{P}_\circ^2 - \frac{\sqrt{3}}{3}K_\circ \frac{\Pi_A}{A} \quad (4.70)$$

and the ensuing canonical system,

$$\dot{A} = -\frac{\sqrt{3}}{3}N \frac{K_\circ}{A}, \quad (4.71a)$$

$$\dot{K}_\circ = \frac{1}{3}N A \mathcal{P}_\circ, \quad (4.71b)$$

$$\dot{\Pi}_A = -N \left(\frac{1}{6} \mathcal{P}_\circ^2 + \frac{\sqrt{3}}{3} K_\circ \frac{\Pi_A}{A^2} \right), \quad (4.71c)$$

$$\dot{\mathcal{P}}_\circ = \frac{\sqrt{3}}{3}N \frac{\Pi_A}{A}, \quad (4.71d)$$

²³We prefer not to write down the details of the resolution since this is not a very exciting task.

possesses two first integrals: $\Pi_A = aA^2$ and $A\Pi_A + K_o\mathcal{P}_o = b$, with a and b constant.

When the scalar curvature is not constant we choose $R = \rho e^t$ and straightly integrate the canonical system to obtain the general solution in the form

$$ds^2 = -\frac{e^{2t}}{(1 - n_o e^{3t})^2} dt^2 + \frac{dl^2}{(1 - n_o e^{3t})^{\frac{2}{3}}}, \quad (4.72)$$

where n_o is a constant of integration. Therefore we see that this representation coincides with the isotropic limit (4.47) of the Bianchi-type I solution.

On the other hand, if we consider spaces of constant curvature, i.e. $R = 4\Lambda$, then we obtain from the canonical system (4.71) and the super-Hamiltonian constraint (4.70) the elementary differential equation $\dot{A}/A = \pm\omega$, where $\omega^2 := \frac{1}{3}\Lambda$, whence we derive two distinct solutions (up to rescaled coordinates),

$$A(t) = \begin{cases} \Lambda^{-\frac{1}{2}} e^{\pm\sqrt{\Lambda}t} & \text{if } \Lambda > 0, \\ |\Lambda|^{-\frac{1}{2}} \cos(\sqrt{|\Lambda|}t) & \text{if } \Lambda < 0, \end{cases} \quad (4.73)$$

which correspond respectively to a de Sitter space and an anti-de Sitter space. This exemplifies the relevance of the R -squared theory to the inflationary scenario: In the field equations the terms that come specifically from the quadratic part of the Lagrangian density can play the rôle of a cosmological constant; moreover it is well known that the addition of the R^2 term in the gravitational action introduces a new spin-0 scalar field which may act as a natural inflaton in the early universe (cf. the Introduction).

For a zero scalar curvature the canonical equations are easily integrated and we obtain the solution $ds^2 = -dt^2 + tdl^2$, which was found independently by Caprasse et al. from a search of Groebner bases of the system of algebraic equations associated with power-law type solutions of the fourth-order field equations [CDGM91].

4.3.3 Conformal Bianchi-type I model

Canonical equations and super-Hamiltonian

In conformal gravity the canonical action (4.25) reduces to

$$S = \int dt \left[\Pi_\mu \dot{\mu} + \Pi_\pm \dot{\beta}_\pm + \mathcal{P}_\pm \dot{K}_\pm - N\mathcal{H} \right], \quad (4.74)$$

owing to the existence of the primary constraint (3.186), which translates into $\mathcal{P}_o \approx 0$ in terms of the new variables introduced on page 147. The explicit form of the super-Hamiltonian constraint depends on the Bianchi type considered; for type IX,

for instance, this is given by the expression (4.26) without those few terms involving \mathcal{P}_\circ . In the action (4.74) we have not written the super-momentum constraints since they identically vanish for all diagonal class A models but type VI₀; we also reiterate that the surface terms at spatial infinity arising in the canonical formalism come to naught when one considers space-time isometries corresponding to spatially homogeneous Bianchi cosmologies (cf. the discussion on boundary terms on pages 131–132).

We focus on the simplest cosmological model that exhibits nontrivial degrees of freedom in conformal gravity, i.e. Bianchi type I—the isotropic FLRW space-times are conformally flat. In this case the super-Hamiltonian is

$$\begin{aligned} \mathcal{H} = & \frac{\sqrt{6}}{6} \left[4\mathcal{P}_- K_+ K_- - 2\mathcal{P}_+ (K_+^2 - K_-^2) - K_\pm \Pi_\pm \right] \\ & + \frac{\sqrt{3}}{3} K_\circ (K_\pm \mathcal{P}_\pm - \Pi_\mu) - \frac{1}{2} e^{-3\mu} (\mathcal{P}_+^2 + \mathcal{P}_-^2). \end{aligned} \quad (4.75)$$

(The coupling constant α of the Weyl-squared term has been set equal to one.)

We apply the Dirac–Bergmann consistency algorithm to this constrained system. The Dirac Hamiltonian density is $\mathfrak{H}_\mathcal{D} = N\mathcal{H} + \lambda_\circ \mathcal{P}_\circ$, with a Lagrange multiplier λ_\circ . Conservation of the primary constraint $\mathcal{P}_\circ \approx 0$ brings forth the secondary constraint $\chi_\circ \approx 0$, viz.

$$\mathcal{P}_\circ \approx 0 \longrightarrow \chi_\circ = \Pi_\mu - K_\pm \mathcal{P}_\pm \approx 0.$$

Since we have the zero Poisson bracket $\{\mathcal{P}_\circ, \chi_\circ\} \approx 0$ the above primary and secondary constraints are first class (the secondary one is the generator of conformal transformations). To proceed we must impose a gauge-fixing condition associated with the ‘conformal constraint’ $\chi_\circ \approx 0$. We introduce the coordinate condition $\mu \approx 0$ as an additional (primary) constraint—this amounts to turning the conformal constraint into second class. Conservation of this additional constraint yields the secondary constraint $K_\circ \approx 0$. Therefore we end up with a set of four constraints, which are obviously second class. This enables one to eliminate the pairs of canonical variables $\{\mu, \Pi_\mu\}$ and $\{K_\circ, \mathcal{P}_\circ\}$. The canonical action (4.74) reduces to

$$S = \int dt \left[\Pi_\pm \dot{\beta}_\pm + \mathcal{P}_\pm \dot{K}_\pm - \mathcal{H} \right], \quad (4.76)$$

where, in accordance with the conformal invariance of the theory and the form of the Bianchi metrics (4.24), we have parameterised the lapse function as $N = e^\mu$; hence the gauge fixing described above amounts to choosing a specific conformal factor for the type I metric. The super-Hamiltonian constraint (4.75) now reduces

to

$$\mathcal{H} = \frac{\sqrt{6}}{6} \left[4\mathcal{P}_- K_+ K_- - 2\mathcal{P}_+ (K_+^2 - K_-^2) - K_\pm \Pi_\pm \right] - \frac{1}{2} (\mathcal{P}_+^2 + \mathcal{P}_-^2). \quad (4.77)$$

Varying the action (4.76) with respect to the canonical variables and conjugate momenta we obtain the canonical equations of Bianchi type I in conformal gravity:

$$\dot{\beta}_\pm = -\frac{\sqrt{6}}{6} K_\pm, \quad (4.78a)$$

$$\dot{\Pi}_\pm = 0, \quad (4.78b)$$

$$\dot{K}_+ = \frac{\sqrt{6}}{3} (K_-^2 - K_+^2) - \mathcal{P}_+, \quad (4.78c)$$

$$\dot{K}_- = \frac{2\sqrt{6}}{3} K_+ K_- - \mathcal{P}_-, \quad (4.78d)$$

$$\dot{\mathcal{P}}_+ = \frac{\sqrt{6}}{6} (\Pi_+ - 4K_- \mathcal{P}_- + 4K_+ \mathcal{P}_+), \quad (4.78e)$$

$$\dot{\mathcal{P}}_- = \frac{\sqrt{6}}{6} (\Pi_- - 4K_- \mathcal{P}_+ - 4K_+ \mathcal{P}_-). \quad (4.78f)$$

This system supplemented with the super-Hamiltonian constraint (4.77) is equivalent to the Bach equations $B_{ab} = 0$. (The components of the Bach tensor B_{ab} are written down in the Appendix at the end of this section on page 175 ff.) We have indeed explicitly checked that: (i) the canonical equations (4.78b) are in fact the (spatial) Euler-Lagrange equations, i.e. $B_{ii} = 0$ for $i = 1, 2, 3$, derived from the conformal quadratic action, owing to the recursion relations for the momenta Π_\pm that are obtained from equations (4.78e) and (4.78f);²⁴ (ii) the super-Hamiltonian constraint (4.77) coincides exactly with the ‘time-time’ component of the Bach tensor, i.e. $B_{00} = 0$.

Having at our disposal—instead of the Bach equations—the nice differential system (4.78) and the algebraic constraint (4.77) we intend to seek out exact solutions by performing a global involution algorithm on appropriate extra constraints that yield closed constraint algebras.

Global involution algorithm

The involution method consists in applying the Dirac–Bergmann consistency algorithm to our classical system, with the Poisson bracket defined with respect to the canonical variables β_\pm , Π_\pm , K_\pm , \mathcal{P}_\pm , and after suitable conditions, i.e. additional

²⁴This equivalence is best understood with a glance at the box on page 76.

ad hoc constraints, have been imposed.²⁵ Strictly speaking, the steps of the global involution algorithm are:

1. Impose an appropriate extra constraint on the canonical variables.
2. Require that this constraint be preserved when time evolution is considered. This gives rise to secondary constraints and possibly to the determination of the Lagrange multiplier associated with the extra constraint.
3. Repeat Step (2) until no new information comes out.

Once the involution algorithm has been performed we may classify all the constraints into first class and second class and proceed further to the analysis of the particular system.

Constraint $\varphi_k \approx 0$. The first extra constraint we consider expresses that the ratio of the variables K_{\pm} be constant, namely

$$\varphi_k^{(0)} = K_- - kK_+ \approx 0, \quad k \in \mathbb{R}. \quad (4.79)$$

The Poisson bracket of $\varphi_k^{(0)}$ and \mathcal{H} yields the secondary constraint

$$\varphi_k^{(1)} = \frac{\sqrt{6}}{3}k(k^2 - 3)K_+^2 + (\mathcal{P}_- - k\mathcal{P}_+) \approx 0. \quad (4.80)$$

The Poisson bracket of $\varphi_k^{(1)}$ and the Dirac Hamiltonian density $\mathcal{H}_{\mathcal{D}} := \mathcal{H} + \lambda_k \varphi_k^{(0)}$ leads to the determination of the Lagrange multiplier, viz. $\lambda_k \approx \sqrt{6}(\Pi_- - k\Pi_+)/[6(1 + k^2)]$, which turns out to be constant, and the algorithm stops. Both constraints (4.79) and (4.80) are second class since their Poisson bracket is equal to $1 + k^2$. Thus we can eliminate the corresponding spurious degrees of freedom. To this end we perform the canonical transformation

$$\mathcal{P}_+ \longrightarrow \frac{\mathcal{P}_+ - k\mathcal{P}_-}{1 + k^2}, \quad \mathcal{P}_- \longrightarrow \frac{k\mathcal{P}_+ + \mathcal{P}_-}{1 + k^2}. \quad (4.81)$$

The action (4.76) then reduces to

$$S = \int dt \left[\Pi_{\pm} \dot{\beta}_{\pm} + \mathcal{P}_+ \dot{K}_+ - \mathcal{H}' \right], \quad (4.82)$$

where the super-Hamiltonian (4.77) is now given by

$$\begin{aligned} \mathcal{H}' = & \frac{k^2(k^2 - 3)^2}{3(1 + k^2)}K_+^4 + \frac{\sqrt{6}(3k^2 - 1)}{3(1 + k^2)}K_+^2\mathcal{P}_+ \\ & - \frac{\sqrt{6}}{6}(\Pi_+ + k\Pi_-)K_+ - \frac{\mathcal{P}_+^2}{2(1 + k^2)}. \end{aligned} \quad (4.83)$$

²⁵For a rigorous treatment on the concept of involution as applied to constrained systems, we refer the interested reader to Seiler and Tucker's article [ST95] (see also [Ger96]).

Varying the action (4.82) with respect to the pair of canonical variables K_+ and \mathcal{P}_+ we obtain the canonical equations

$$\dot{K}_+ = \frac{\sqrt{6}(3k^2 - 1)}{3(1 + k^2)} K_+^2 - \frac{\mathcal{P}_+}{1 + k^2}, \quad (4.84a)$$

$$\dot{\mathcal{P}}_+ = \frac{4k^2(k^2 - 3)^2}{3(1 + k^2)^2} K_+^3 + \frac{2\sqrt{6}(3k^2 - 1)}{3(1 + k^2)} K_+ \mathcal{P}_+ - \frac{\sqrt{6}}{6} (\Pi_+ + k\Pi_-). \quad (4.84b)$$

Taking into account the explicit form of the super-Hamiltonian (4.83) we obtain a nonlinear first-order differential equation for $K_+(t)$,

$$\dot{K}_+^2 = \frac{2}{3}(1 + k^2)K_+^4 - \frac{\sqrt{6}(\Pi_+ + k\Pi_-)}{3(1 + k^2)} K_+, \quad (4.85)$$

which can be written as one binomial equation of Briot and Bouquet,

$$\dot{u}^2 = u^4 + \gamma^3 u, \quad (4.86)$$

in terms of a new variable u defined by the homography $u = \pm \frac{\sqrt{6}}{3} K_+ \sqrt{1 + k^2}$, and with $\gamma^3 = \mp \frac{2}{3} (\Pi_+ + k\Pi_-) (1 + k^2)^{-1/2}$. Direct calculation shows that its general solution is given by

$$u(t) = \frac{\gamma^3}{4\mathcal{W}}, \quad (4.87)$$

where \mathcal{W} stands for the Weierstrass elliptic function $\wp(t - t_0; g_2, g_3)$, with invariants $g_2 = 0$ and $g_3 = -\frac{1}{36} (\Pi_+ + k\Pi_-)^2 / (1 + k^2)$, and with one arbitrary constant t_0 (cf. [AS65, p. 627 ff.]). In terms of the canonical pair (K_+, \mathcal{P}_+) the representation (4.87) corresponds to the expressions

$$K_+(t) = -\frac{\sqrt{6}(\Pi_+ + k\Pi_-)}{12(1 + k^2)} \frac{1}{\mathcal{W}}, \quad (4.88a)$$

$$\mathcal{P}_+(t) = -\frac{\sqrt{6}(\Pi_+ + k\Pi_-)}{72\mathcal{W}^2} \left[\frac{1 - 3k^2}{(1 + k^2)^2} (\Pi_+ + k\Pi_-) + 6\mathcal{W} \frac{d \ln \mathcal{W}}{dt} \right], \quad (4.88b)$$

where

$$\mathcal{W} \frac{d \ln \mathcal{W}}{dt} = \pm \frac{1}{6} \sqrt{144\mathcal{W}^3 + \frac{(\Pi_+ + k\Pi_-)^2}{1 + k^2}}.$$

To obtain the analytic form of the anisotropic metric functions $\beta_{\pm}(t)$ we must integrate the right-hand side of equation (4.88a). We apply the following result [AS65, p. 641].²⁶

²⁶ A prime denotes differentiation with respect to z , the argument of the Weierstrassian functions considered hereafter.

Proposition 4.3.1. *If $\wp'(z_0) \neq 0$, then*

$$\wp'(z_0) \int \frac{dz}{\wp(z) - \wp(z_0)} = 2z \zeta(z_0) + \ln \sigma(z - z_0) - \ln \sigma(z + z_0),$$

with Weierstrassian functions $\zeta(z)$ and $\sigma(z)$ defined by $\zeta'(z) + \wp(z) = 0$ and $\sigma'(z) - \sigma(z)\zeta(z) = 0$ respectively.

To achieve our aim we take $z = t$ and $z_0 = t_z$, where t_z is a zero of the Weierstrass elliptic function, i.e. $\wp(t_z) = 0$. Indeed, we obtain

$$\int \frac{dt}{\mathcal{W}(t)} = \pm \frac{6\sqrt{1+k^2}}{\Pi_+ + k\Pi_-} [2t \zeta(t_z) + \ln \sigma(t - t_z) - \ln \sigma(t + t_z)] \quad (4.89)$$

and we can write the corresponding homogeneous metrics of type I under the form

$$\begin{aligned} ds^2 = & -dt^2 + \exp \left[\pm \frac{2(1+\sqrt{3}k)}{\sqrt{1+k^2}} t \zeta(t_z) \right] \left[\frac{\sigma(t - t_z)}{\sigma(t + t_z)} \right]^{\pm \frac{1+\sqrt{3}k}{\sqrt{1+k^2}}} dx^2 \\ & + \exp \left[\pm \frac{2(1-\sqrt{3}k)}{\sqrt{1+k^2}} t \zeta(t_z) \right] \left[\frac{\sigma(t - t_z)}{\sigma(t + t_z)} \right]^{\pm \frac{1-\sqrt{3}k}{\sqrt{1+k^2}}} dy^2 \\ & + \exp \left[\mp \frac{4}{\sqrt{1+k^2}} t \zeta(t_z) \right] \left[\frac{\sigma(t - t_z)}{\sigma(t + t_z)} \right]^{\mp \frac{2}{\sqrt{1+k^2}}} dz^2. \end{aligned} \quad (4.90)$$

As a particular case of the present analysis we can specialise the above solution (4.87) to the axisymmetric case, for which the secondary constraint (4.80) reduces to the conditions

$$\frac{K_-}{K_+} \approx k \approx \frac{\mathcal{P}_-}{\mathcal{P}_+}, \quad k \in \{0, \pm\sqrt{3}\}. \quad (4.91)$$

According to the canonical transformation (4.81) the new variable \mathcal{P}_- vanishes automatically. The super-Hamiltonian (4.83) becomes

$$\mathcal{H}'_{\text{axi}} = \frac{\sqrt{6}(3k^2 - 1)}{3(1 + k^2)} K_+^2 \mathcal{P}_+ - \frac{\sqrt{6}}{6} (\Pi_+ + k\Pi_-) K_+ - \frac{\mathcal{P}_+^2}{2(1 + k^2)}. \quad (4.92)$$

and the corresponding canonical equations are

$$\dot{K}_+ = \frac{\sqrt{6}(3k^2 - 1)}{3(1 + k^2)} K_+^2 - \frac{\mathcal{P}_+}{1 + k^2}, \quad (4.93a)$$

$$\dot{\mathcal{P}}_+ = \frac{2\sqrt{6}(3k^2 - 1)}{3(1 + k^2)} K_+ \mathcal{P}_+ - \frac{\sqrt{6}}{6} (\Pi_+ + k\Pi_-). \quad (4.93b)$$

As in the general case we find out the binomial equation of Briot and Bouquet (4.85), the solution (4.87) of which is valid for any value of the parameter k ; hence the axisymmetric solution is obtained by setting k to 0 or $\pm\sqrt{3}$ in expressions (4.88) and finally in the metric (4.90).

Constraint $\varphi_p \approx 0$. Consider the extra constraint expressing that the ratio of the variables \mathcal{P}_\pm be constant, namely

$$\varphi_p^{(0)} = \mathcal{P}_- - p\mathcal{P}_+ \approx 0, \quad p \in \mathbb{R}. \quad (4.94)$$

The Poisson bracket of $\varphi_p^{(0)}$ and $\mathcal{H}_\mathcal{D} := \mathcal{H} + \lambda_p \varphi_p^{(0)}$ yields the secondary constraint

$$\varphi_p^{(1)} = 4\mathcal{P}_+ [K_-(p^2 - 1) - 2pK_+] + (\Pi_- - p\Pi_+) \approx 0. \quad (4.95)$$

To check the consistency of the involution algorithm we consider two distinct cases:

1. The secondary constraint (4.95) is identically satisfied if $\Pi_- - p\Pi_+ \approx 0$ and $K_-(p^2 - 1) - 2pK_+ \approx 0$. Again, in order to proceed, we split up the analysis into two subdivisions:

- (a) If $p \neq \sigma$, with $\sigma = \pm 1$, the following weak equality holds: $K_- \approx 2pK_+/(p^2 - 1)$. The Poisson bracket of $\varphi_p^{(1)}$ and $\mathcal{H}_\mathcal{D}$ yields the constraint

$$\begin{aligned} \varphi_p^{(2)} &= (1 - 3p^2)\lambda_p - p(p^2 - 3)\mathcal{P}_+ \\ &\quad - \frac{2\sqrt{6}p(1 - 3p^2)(p^2 - 3)}{3(p^2 - 1)^2} K_+^2 \approx 0, \end{aligned} \quad (4.96)$$

where $p \neq \frac{\sigma}{\sqrt{3}}$ since we consider nonzero canonical variables \mathcal{P}_\pm . Consistency then leads to the determination of the Lagrange multiplier λ_p , viz.

$$\lambda_p \approx \frac{2\sqrt{6}p(p^2 - 3)}{3(p^2 - 1)^2} K_+^2 - \frac{p(p^2 - 3)}{3p^2 - 1} \mathcal{P}_+.$$

When $p \in \{0, \sigma\sqrt{3}\}$ the Poisson bracket of $\varphi_p^{(2)}$ and $\mathcal{H}_\mathcal{D}$ vanishes identically and the involution algorithm does not generate any new constraints. This subcase corresponds to a particular case of the axisymmetric solution with $k = p$ and $\Pi_- \approx p\Pi_+$ (cf. equation (4.91)). For the nonaxisymmetric case, on the other hand, the next step in the involution algorithm yields

$$\Pi_+ \approx \left[\frac{8\sqrt{6}(3p^2 - 1)(p^2 + 1)}{3(p + 1)^3(p - 1)^3} K_+^2 - \frac{4(p^2 + 1)}{p^2 - 1} \mathcal{P}_+ \right] K_+$$

and the last step gives

$$\mathcal{P}_+ \approx \frac{\sqrt{6}(1 - 3p^2)(\sigma - 3)}{6(p^2 - 1)^2} K_+^2.$$

At this stage no more constraints arise. Taking into account that the super-Hamiltonian (4.77) is weakly vanishing we find out that Π_+ must be equal to zero. This subcase will be discussed below, as part of our discussion on the generic case with $\Pi_\pm \approx 0$.

- (b) If $p = \sigma$, then K_+ is weakly vanishing. The Poisson bracket of $\varphi_p^{(1)}$ and $\mathcal{H}_{\mathcal{D}}$ yields the constraint

$$\varphi_p^{(2)} = \lambda_p - \sigma \mathcal{P}_+ + \frac{\sqrt{6}\sigma}{3} K_-^2 \approx 0 \quad (4.97)$$

and consistency determines the Lagrange multiplier λ_p . The Poisson bracket of $\varphi_p^{(2)}$ and $\mathcal{H}_{\mathcal{D}}$ gives the weak equality

$$\Pi_+ \approx \frac{4}{\sigma} \left(\frac{\sqrt{6}}{3} K_-^2 - \mathcal{P}_+ \right) K_-.$$

The last step in the involution algorithm yields

$$\mathcal{P}_+ \approx \frac{\sqrt{6}}{12} (3 + \sigma) K_-^2.$$

At this stage no more constraints arise. The vanishing of the super-Hamiltonian (4.77) restricts Π_+ to be zero. As in the previous nonaxisymmetric case with $p \neq \sigma$, this subcase will be discussed below.

2. When $\Pi_- - p\Pi_+ \neq 0$, the Poisson bracket of $\varphi_p^{(1)}$ and $\mathcal{H}_{\mathcal{D}}$ yields the constraint

$$\begin{aligned} \varphi_p^{(2)} = & \sqrt{6}p(p^2 - 3)\mathcal{P}_+^2 - \sqrt{6}(1 - 3p^2)\lambda_p\mathcal{P}_+ \\ & - 4\mathcal{P}_+(K_+ + pK_-)(pK_+ - K_-) \\ & + \Pi_-(K_+ - pK_-) + \Pi_+(pK_+ + K_-) \approx 0. \end{aligned}$$

If $p = \frac{\sigma}{\sqrt{3}}$, the involution algorithm closes when $\varphi_p^{(5)}$ is computed, but it does not lead to any exact solutions since the super-Hamiltonian is not compatible with the constraints $\varphi_p^{(j)}$ for $j = 1, \dots, 5$. On the other hand, if $p \neq \frac{\sigma}{\sqrt{3}}$, we have not been able to close the algorithm. It turns out, however, that the involution algorithm in this case is useless since the system under consideration does not produce an integration case, as it can be shown by a local study of its analytic structure [DQS98].²⁷

Constraints $\Pi_{\pm} \approx 0$. Consider now the extra constraints expressing that the canonical variables Π_{\pm} be equal to zero. Contrary to the involution of the previous constraints φ_k and φ_p , the consistency algorithm here is trivial: it is unable to produce any new information since there are no secondary constraints. The constraints $\Pi_{\pm} \approx 0$ are first class; we can choose their corresponding Lagrange multipliers λ_{\pm} to be zero. In that case the constraints remain weak equations to be imposed on the physical states of the system. Hence, at the classical level, the

²⁷Strictly speaking, the system with the constraint (4.94) does not possess the Painlevé property.

appropriate system of canonical equations is the system (4.78), where we set Π_{\pm} to zero. Besides equation (4.78a), the relevant equations are thus

$$\dot{K}_+ = \frac{\sqrt{6}}{3}(K_-^2 - K_+^2) - \mathcal{P}_+, \quad (4.98a)$$

$$\dot{K}_- = \frac{2\sqrt{6}}{3}K_+K_- - \mathcal{P}_-, \quad (4.98b)$$

$$\dot{\mathcal{P}}_+ = \frac{2\sqrt{6}}{3}(K_+\mathcal{P}_+ - K_-\mathcal{P}_-), \quad (4.98c)$$

$$\dot{\mathcal{P}}_- = -\frac{2\sqrt{6}}{3}(K_-\mathcal{P}_+ + K_+\mathcal{P}_-). \quad (4.98d)$$

The super-Hamiltonian (4.77) is now given by

$$\mathcal{H} = \frac{\sqrt{6}}{3} \left[2\mathcal{P}_-K_+K_- - \mathcal{P}_+(K_+^2 - K_-^2) \right] - \frac{1}{2}(\mathcal{P}_+^2 + \mathcal{P}_-^2). \quad (4.99)$$

The general solution of equations (4.98) is easy to produce under closed analytic form. We first solve equations (4.98a) and (4.98b) for \mathcal{P}_+ and \mathcal{P}_- respectively and write down second-order equations for K_+ and K_- , namely

$$3\ddot{K}_{\pm} = 4\Sigma K_{\pm}, \quad \text{with } \Sigma := K_+^2 + K_-^2. \quad (4.100)$$

Aside from the super-Hamiltonian constraint, the canonical system (4.98) possesses the first integral

$$K_+\dot{K}_- - K_-\dot{K}_+ = \delta, \quad (4.101)$$

where δ is an arbitrary constant. This first integral has been found independently from a direct analysis of the Bianchi-type I field equations in conformal gravity [Rem98]. Making use of the super-Hamiltonian constraint (4.99) we produce a scalar second-order equation for Σ , namely $\ddot{\Sigma} = 4\Sigma^2$. We integrate this equation and obtain the solution $2\Sigma = 3\wp(t - t_0; 0, g_3)$, with arbitrary constants t_0 and $g_3 = \frac{16}{9}\delta^2$. This reduces the system (4.100) to linear differential equations of the Lamé type, i.e.

$$\ddot{K}_{\pm} = 2\wp(t - t_0; 0, g_3)K_{\pm},$$

which are studied exhaustively in [Inc44, WW50]. If we adopt Ince's notations, our particular case of the Lamé equation is specified by $h = 0$ and $n = 1$.²⁸ If we introduce t_z such that the transcendental equation $\wp(t_z) = 0$ is satisfied, i.e. t_z is

²⁸The general solution to the system (4.98) is uniform; this confirms the single-valuedness of a possible integrability case detected by the Painlevé test: the complete system with $\Pi_{\pm} = 0$ has the Painlevé property [DQS98].

a zero of the Weierstrass elliptic function, then the general solution to the system under study is given by the fundamental set

$$K_{\pm,1} = \exp[-t \zeta(t_z)] \frac{\sigma(t + t_z)}{\sigma(t)}, \quad (4.102a)$$

$$K_{\pm,2} = \exp[+t \zeta(t_z)] \frac{\sigma(t - t_z)}{\sigma(t)}, \quad (4.102b)$$

with Weierstrassian functions $\zeta(t)$ and $\sigma(t)$ defined by $\dot{\zeta}(t) + \wp(t) = 0$ and $\dot{\sigma}(t) - \sigma(t)\zeta(t) = 0$ respectively. The solutions given by the fundamental set (4.102) are distinct, provided that the parameters e_i for $i = 1, 2, 3$, which are defined by

$$e_1 + e_2 + e_3 = 0, \quad 4(e_2 e_3 + e_3 e_1 + e_1 e_2) = -g_2 \equiv 0, \quad 4e_1 e_2 e_3 = g_3,$$

are not equal to zero; this is indeed the case here whenever $g_3 \neq 0$. If $g_3 = 0 = \delta$, then $e_1 = e_2 = e_3 = 0$ and the solutions in the fundamental set are one and the same.²⁹

$$K_+ = \pm \frac{\sqrt{6} \sin 4K}{2} \frac{1}{t - t_0}, \quad (4.103a)$$

$$K_- = \frac{\sqrt{6} \cos 4K}{2} \frac{1}{t - t_0}, \quad (4.103b)$$

$$\mathcal{P}_+ = \frac{\sqrt{6}}{2} \frac{1 \pm \sin 4K - 2 \sin^2 4K}{(t - t_0)^2}, \quad (4.103c)$$

$$\mathcal{P}_- = \frac{\sqrt{6} \cos 4K}{2} \frac{(1 \pm 2 \sin 4K)}{(t - t_0)^2}, \quad (4.103d)$$

with K constant. Denoting $\chi := t - t_0$ and integrating equations (4.78a) we obtain type I homogeneous metrics under the form

$$ds^2 = -d\chi^2 + \sum_{i=1}^3 \chi^{2\nu_i} (dx^i)^2, \quad (4.104)$$

where the parameters ν_i for $i = 1, 2, 3$ satisfy the relations

$$\sum_{i=1}^3 \nu_i = 0, \quad \sum_{i=1}^3 \nu_i^2 = \frac{3}{2}.$$

²⁹This case is better understood in the light of its analytic structure: it turns out that one of the relevant singularity families of our general canonical system becomes an exact two-parameter particular solution when Π_{\pm} vanish [DQS98].

Analytic structure of the Bianchi-type I system

The Painlevé strategy. The existence of the above solutions, whether particular solutions of the general differential system or general solutions of specialised systems, tells nothing about the integrability or non-integrability of the complete system and gives no information whatsoever about the mere accessibility of an exact and closed-form analytic expression of its general solution. This is due to the fact that the global involution algorithm of the extra constraints, as operated above, is not related with integrability and may even prove to be nonexhaustive. The integrability issue is tackled through an invariant investigation method of intrinsic properties of the general solution. In particular, the result does not depend on specific choices of the metric, within some well-defined equivalence class.

The approach advocated by Painlevé proceeds from the main observation, nowadays frequently exemplified in various areas of theoretical physics, that all analytic solutions encountered are single-valued or multiple-valued *finite* expressions (possibly intricate) depending on a finite number of *functions*—solutions of linear equations, elliptic functions, and the six transcendental functions systematically extracted by Painlevé and Gambier. Therefore, the building blocks of this process are the functions, which are explicitly defined through their single-valuedness. This emphasises the relevance of the analytic structure of the solution, as uniformisability ensures adaptability to all possible sets of initial conditions. The next step of this approach deals with integrability in some fundamental sense. Indeed, probing the analytic structure of a system requires a global, as opposed to local, integrability-related property, namely the *Painlevé property*.³⁰ At this level, integrable systems are defined in the sense of Painlevé as those systems that possess the Painlevé property.³¹ Moreover, in keeping with the above observation, the requirement for global single-valuedness ought to be relaxed to accommodate this definition to integrability in the practical sense. Upon using broader classes of transformations, the (unavoidable) analytic structure of the solution is easily kept under control and either allows or rules out the possibility to produce a mode of representation of the general integral.

Such an approach requires the analytic continuation of the solution in the complex domain of the independent variable and computes generic behaviours of the solution in a vicinity of each movable singularity. The trivial part of the

³⁰A differential system possesses this property if, and only if, its general solution is uniformisable or, equivalently, exhibits no movable critical singularity.

³¹The Painlevé property is invariant under arbitrary holomorphic transformations of the independent variable and arbitrary homographic transformations of dependent variables. In particular, the results given in greater detail in [DQS98] are invariant under arbitrary analytic reparameterisations of time.

Painlevé method, known as the Painlevé test, produces necessary but not sufficient conditions for a system to enjoy the Painlevé property and requires local single-valuedness of the general solution in a vicinity of all possible families of movable singularities.³²

Analytic proof of non-integrability. In [DQS98] we have shown that the complete differential system (4.78) admits three distinct local leading behaviours in some vicinity of movable singularities, that is, three distinct singularity families. The first leading behaviour, denoted $f_{(1)}$, is valid in a vicinity of the movable point $t = t_1$ and exists only when $\Pi_+ \Pi_- \neq 0$. The existence of the second singularity family, referred to as $f_{(2),\pm}$, valid in some vicinity of the movable point $t = t_2$, requires $\Pi_-(2\sqrt{3}\Pi_- \pm 3\Pi_+) \neq 0$. The third and last leading behaviour, denoted $f_{(3),\pm}$, is valid in some vicinity of the movable point $t = t_3$ and is associated with another arbitrary constant parameter, denoted K in [DQS98]; moreover it exists only when $4K \notin \{0, \pi, -\pi, \frac{\pi}{2}, -\frac{\pi}{2}, \mp\frac{\pi}{6}, \mp\frac{5\pi}{6}\}$. The super-Hamiltonian (4.77) introduces no new restrictions since, at leading order in $\chi := t - t_i$ for all $i = 1, 2, 3$, it always vanishes in some vicinity of movable singularities around which leading behaviours $f_{(1)}$, $f_{(2),\pm}$, and $f_{(3),\pm}$ hold.

Around each species of movable singularities one must inquire whether it is possible to generate *single-valued generic* local representations of the general solution. The Fuchsian indices have been computed for each leading behaviour and all preliminary conditions have proved to be fulfilled. However, near both movable points t_2 and t_3 in \mathbb{C} , it is not possible to build single-valued generic local expansions, unless some constraints are imposed. Upon introducing movable logarithmic terms in these local series one may regain genericity—at the expense of losing the Painlevé property.³³

Such multiple-valuedness, betrayed by local investigations, also pertains to the general solution itself. This analytically proves that the system under consideration is not integrable: Its general solution exhibits, in complex time, an infinite number of logarithmic transcendental essential movable singularities; in other words, an analytic structure not compatible with integrability in the practical sense—the quest for generic, exact and closed-form analytic expressions of the solution is hopeless. This result holds under space-time transformations within the equivalence class of the Painlevé property; see [Con99]. Yet, local information produced by the Painlevé

³²Movable essential singularities are difficult to handle, since one lacks methods to write down conditions under which they are indeed noncritical. For a tutorial presentation of basic ideas and constructive algorithms aimed at the generation of integrability conditions, we refer the interested reader to [Con99, RGB89].

³³For a thorough account and a complete proof of these claims, cf. [DQS98, Appendix B].

test may still be used in order to extract all particular systems that may prove to be integrable. In the case under study, it turns out that all particular solutions are meromorphic, but this is only a result of the application of the method.

All integrable particular cases. Even though this does not provide a proof but merely an indication of uniformisability, the Painlevé test requires local single-valuedness around all possible species of movable singularities. Utilising the results obtained from the Painlevé analysis [DQS98, Appendix B] and comparing them with those derived from the global involution algorithm above we draw the following conclusions:

- Near the movable point $t = t_2$, the complete set of integrability conditions is satisfied if one imposes $\Pi_- = \pm\sqrt{3}\Pi_+$ and simultaneously requires the vanishing of the arbitrary constant parameter associated with the index $j = -3$. On the other hand, if one sets $2\sqrt{3}\Pi_- = \mp 3\Pi_+$ or $\Pi_- = 0$, the family $f_{(2),\pm}$ dies out and *ipso facto* no restriction needs fulfilment.
- Near the movable point $t = t_3$, single-valuedness may only be recovered in two particular cases. The first case deals with a local representation of the general solution of that specialised system obtained with $\Pi_{\pm} = 0$. In this case local leading behaviours $f_{(1)}$ and $f_{(2),\pm}$ die out whereas, near $t = t_3$, a meromorphic local generic expansion is produced. This corresponds to the closed-form solution (4.102). The second case deals with a local representation of some particular solution of the complete differential system and requires that the arbitrary parameter K be such that $\sin 4K = \Pi_+(\Pi_+^2 + \Pi_-^2)^{-1/2}$ and $\cos 4K = \pm\Pi_-(\Pi_+^2 + \Pi_-^2)^{-1/2}$.
- The closed-form solution (4.90) obtained by imposing the extra constraint $\varphi_k \approx 0$ on the system corresponds to one particular integrable case, for it turns out that:
 1. all indices that characterise the $f_{(3),\pm}$ singularity family are compatible;
 2. the $f_{(2),\pm}$ singularity family dies out unless $k \in \{0, \pm\sqrt{3}\}$, but in this latter instance the indices are compatible.
- The particular axisymmetric solution with $\mathcal{P}_- = \pm\sqrt{3}\mathcal{P}_+$ corresponds to the integrable case of the $f_{(2),\pm}$ singularity family.
- The closed-form solution (4.104) corresponds to the case when the singularity family $f_{(3),\pm}$ becomes an exact two-parameter solution whenever $\Pi_{\pm} = 0$.

These results clearly indicate that the global involution algorithm of extra constraints has proven to be exhaustive in the search for exact solutions that may be written in closed analytical form.

Conformal relationship with Einstein spaces

The problem of conformal relationship between Riemannian spaces and Einstein spaces was first addressed circa 1920 by Brinkmann who studied the necessary and sufficient conditions for n -dimensional spaces to be conformally related to Einstein spaces [Bri24, Bri25].³⁴ Kozameh, Newman, and Tod reexamined this question for four-dimensional manifolds and obtained nice results by addressing the problem at one and the same time from the tensor and spinor points of view [KNT85].³⁵

In the context of conformal gravity it is crucial to determine whether closed-form solutions are conformally related to Einstein spaces or not: Since every Einstein space or every space conformal to an Einstein space fulfils the vacuum Bach equations automatically, any closed-form solution that can be mapped onto an Einstein space can be thought of—from the point of view of generalised gravity theories—as a minor solution; as a matter of fact the interesting solutions will be those that are not conformal to an Einstein space.³⁶

In the case under study, i.e. Bianchi-type I cosmology, despite the fact that the general system is not integrable, as was proven by the Painlevé analysis, we have obtained all the particular exact solutions that may be written in closed analytical form. In keeping with the remark above, it is natural to discuss the conformal relationship of those solutions with Einstein spaces [Que98].

A four-dimensional space-time (\mathcal{M}, g) can be mapped onto an Einstein space under a conformal transformation $\tilde{g}_{ab} = e^{2\sigma(\mathbf{x})}g_{ab}$ if and only if there exists a smooth function $\sigma(\mathbf{x})$ that satisfies

$$L_{ab} = \nabla_a \sigma \nabla_b \sigma - \nabla_a \nabla_b \sigma - \frac{1}{2} g_{ab} g^{cd} \nabla_c \sigma \nabla_d \sigma - \frac{\Lambda}{6} e^{2\sigma} g_{ab}, \quad (4.105)$$

where the tensor L_{ab} is defined by $L_{ab} := \frac{1}{12}(Rg_{ab} - 6R_{ab})$ and $\Lambda := \frac{1}{4}\tilde{R}$ denotes the cosmological constant that characterises the conformal Einstein space (\mathcal{M}, \tilde{g}) [Eis66]. The first integrability conditions of equation (4.105) are given by

$$\nabla_d C^d_{abc} + C^d_{abc} \nabla_d \sigma = 0. \quad (4.106)$$

³⁴Standard results can be found in Schouten's and Eisenhart's textbooks [Sch54, Eis66].

³⁵The very first who undertook this problem within the framework of the spinor formalism was Szekeres [Sze63]; however, the necessary and sufficient conditions he found are extremely difficult to translate into tensorial expressions. By contrast, Kozameh, Newman, and Tod's analysis yields simpler results.

³⁶These are also called 'nontrivial' solutions (according to Schmidt's terminology [Sch84]).

These are the necessary and sufficient conditions for a space to be conformally related to a ‘C-space’, i.e. $\nabla_{[c}L_{b]a} = 0$,³⁷ [Sze63]. The second integrability conditions of equation (4.105) are

$$B_{ab} := 2\nabla^c\nabla^d C_{cabd} + C_{cabd}R^{cd} = 0. \quad (4.107)$$

Therefore, fulfilment of the Bach equations is a necessary condition for a space to be conformally related to an Einstein space. If considered separately the above integrability conditions of equation (4.105) are merely necessary conditions with regard to the conformal relationship with Einstein spaces. However, Kozameh, Newman, and Tod have proven that they constitute a set of sufficient conditions as well [KNT85]:

Theorem 4.3.2. *A space-time (\mathcal{M}, g) is conformally related to an Einstein space (\mathcal{M}, \tilde{g}) if and only if equations (4.106) and (4.107) are fulfilled.*

Specifying equation (4.105) for Bianchi type I we obtain the differential system

$$2\ddot{\sigma} - \dot{\sigma}^2 + 5(\dot{\beta}_+^2 + \dot{\beta}_-^2) - \frac{\Lambda}{3}e^{2\sigma} = 0, \quad (4.108a)$$

$$\dot{\sigma}^2 + 2\dot{\sigma}(\dot{\beta}_+ + \sqrt{3}\dot{\beta}_-) + \ddot{\beta}_+ + \sqrt{3}\ddot{\beta}_- - \dot{\beta}_+^2 - \dot{\beta}_-^2 - \frac{\Lambda}{3}e^{2\sigma} = 0, \quad (4.108b)$$

$$\dot{\sigma}^2 + 2\dot{\sigma}(\dot{\beta}_+ - \sqrt{3}\dot{\beta}_-) - \ddot{\beta}_+ - \sqrt{3}\ddot{\beta}_- - \dot{\beta}_+^2 - \dot{\beta}_-^2 - \frac{\Lambda}{3}e^{2\sigma} = 0, \quad (4.108c)$$

$$\dot{\sigma}^2 - 4\dot{\sigma}\dot{\beta}_+ - 2\ddot{\beta}_+ - \dot{\beta}_+^2 - \dot{\beta}_-^2 - \frac{\Lambda}{3}e^{2\sigma} = 0, \quad (4.108d)$$

which readily integrates to yield the necessary and sufficient condition for a Bianchi-type I space to be conformally related to an Einstein space, namely

$$K_{\pm} = -\sqrt{6}\dot{\beta}_{\pm} = -\sqrt{6}k_{\pm}e^{-2\sigma}, \quad k_{\pm} \neq 0, \quad (4.109)$$

and provides one with a differential equation that enables one to determine explicitly the conformal factor $x := e^{2\sigma}$, viz.

$$\dot{x}^2 = \frac{4}{3}\Lambda x^3 + 4(k_+^2 + k_-^2). \quad (4.110)$$

This last equation can be written as the Weierstrass ordinary differential equation in terms of the Weierstrass elliptic function $\mathcal{W} := \wp(t - t_0; g_2, g_3)$, with invariants $g_2 = 0$ and $g_3 = -\frac{4}{9}\Lambda^2(k_+^2 + k_-^2)$. Therefore, the conformal factor that brings a Bianchi-type I space onto an Einstein space is given by

$$e^{2\sigma(t)} = 3\Lambda^{-1}\mathcal{W}. \quad (4.111)$$

³⁷ There is a natural hierarchy of classes of Riemannian spaces of which the most general class consists of those spaces in which the Bianchi identities take the form $\nabla_d C^d_{abc} = 0$ or, equivalently, $\nabla_{[c}L_{b]a} = 0$; these are called ‘C-spaces’ and contain the Einstein spaces as a subclass [Sze63].

Taking this last result into account we get from equation (4.109) the explicit form of the functions $K_{\pm}(t)$, that is

$$K_{\pm}(t) = -\frac{\sqrt{6}}{3}\Lambda k_{\pm}\mathcal{W}^{-1}. \quad (4.112)$$

So far we have not used the Bach equations nor the equivalent canonical system (4.78). If we do so, we see that the expression (4.112) does actually coincide with the solution (4.88a) upon identifying

$$k \equiv \frac{k_-}{k_+}, \quad \Lambda \equiv \frac{k_+\Pi_+ + k_-\Pi_-}{4(k_+^2 + k_-^2)}. \quad (4.113)$$

Thus we can rewrite type I homogeneous metrics (4.90) under the equivalent form

$$\begin{aligned} ds^2 = & -dt^2 + \exp\left[\pm\frac{2(k_+ + \sqrt{3}k_-)}{\sqrt{k_+^2 + k_-^2}}t\zeta(t_z)\right]\left[\frac{\sigma(t-t_z)}{\sigma(t+t_z)}\right]^{\pm\frac{k_+ + \sqrt{3}k_-}{\sqrt{k_+^2 + k_-^2}}}dx^2 \\ & + \exp\left[\pm\frac{2(k_+ - \sqrt{3}k_-)}{\sqrt{k_+^2 + k_-^2}}t\zeta(t_z)\right]\left[\frac{\sigma(t-t_z)}{\sigma(t+t_z)}\right]^{\pm\frac{k_+ - \sqrt{3}k_-}{\sqrt{k_+^2 + k_-^2}}}dy^2 \\ & + \exp\left[\mp\frac{4k_+}{\sqrt{k_+^2 + k_-^2}}t\zeta(t_z)\right]\left[\frac{\sigma(t-t_z)}{\sigma(t+t_z)}\right]^{\mp\frac{2k_+}{\sqrt{k_+^2 + k_-^2}}}dz^2. \end{aligned} \quad (4.114)$$

This is in agreement with the fact that imposing the constraint (4.79)—here, a direct consequence of equation (4.109)—on the Bach equations is equivalent to requiring the condition (4.106) to be fulfilled, as it can be proved with the help of REDUCE. In other words, assuming that the ratio of variables K_{\pm} be constant is a necessary condition for a Bianchi-type I space to be conformally related to an Einstein space; in conformal gravity, this becomes a sufficient condition as well. Thus the only way to find out a solution to the Bach equations that is not conformally related to an Einstein space is to relax the constraint (4.79). In accordance with our analysis of the preceding sections, we have indeed obtained the only closed-form analytical solution that cannot be mapped onto an Einstein space, namely the general solution (4.102) to the canonical system (4.98), thereby confirming Schmidt's conjecture on the existence of such solutions [Sch84, Que98].

Now examine the particular case of a vanishing cosmological constant. Equation (4.110) becomes trivial and yields (up to an irrelevant constant of integration)

$$e^{2\sigma(t)} = t - t_0 =: \chi. \quad (4.115)$$

Inserting this result into equation (4.109) and integrating we obtain type I homogeneous metrics under the form

$$ds^2 = -d\chi^2 + \chi^{2(k_+ + \sqrt{3}k_-)} dx^2 + \chi^{2(k_+ - \sqrt{3}k_-)} dy^2 + \chi^{-4k_+} dz^2, \quad (4.116)$$

which coincides with the exact two-parameter particular solution (4.104) in the case of zero Π_{\pm} , upon identifying $k_+ \equiv \mp \frac{1}{2} \sin 4K$ and $k_- \equiv -\frac{1}{2} \cos 4K$. Performing a conformal transformation with conformal factor (4.115) and introducing the proper time $\tau := \chi^{3/2}$ we derive the metric (4.116) that characterises the conformal Einstein space with zero cosmological constant, namely

$$ds^2 = -d\tau^2 + \sum_{i=1}^3 \tau^{2p_i} (dx^i)^2, \quad (4.117)$$

where the parameters p_i for $i = 1, 2, 3$ satisfy the relations

$$p_1 + p_2 + p_3 = 1, \quad p_1^2 + p_2^2 + p_3^2 = \frac{1}{3} [1 + 8(k_+^2 + k_-^2)] = 1. \quad (4.118)$$

Hence, as expected, we recover the Bianchi-type I Kasner solution of vacuum general relativity.

Appendix: Bach tensor

We have computed the components of the Bach tensor (2.21) for the Bianchi-type I metric with Misner's parameterisation, utilising the EXCALC package in REDUCE; they are explicitly:

$$\begin{aligned} B_{00} &= 2\ddot{\beta}_- \dot{\beta}_- - \ddot{\beta}_-^2 - 12\dot{\beta}_-^4 - 24\dot{\beta}_-^2 \dot{\beta}_+^2 + 2\ddot{\beta}_+ \dot{\beta}_+ - \ddot{\beta}_+^2 - 12\dot{\beta}_+^4, \\ B_{11} &= \sqrt{3}(\ddot{\beta}_- - 24\ddot{\beta}_- \dot{\beta}_-^2 - 8\ddot{\beta}_- \dot{\beta}_+^2 - 16\dot{\beta}_- \ddot{\beta}_+ \dot{\beta}_+) - 2\ddot{\beta}_- \dot{\beta}_- + \ddot{\beta}_-^2 \\ &\quad - 16\ddot{\beta}_- \dot{\beta}_- \dot{\beta}_+ + 12\dot{\beta}_-^4 - 8\dot{\beta}_-^2 \ddot{\beta}_+ + 24\dot{\beta}_-^2 \dot{\beta}_+^2 + \ddot{\beta}_+ \\ &\quad - 2\ddot{\beta}_+ \dot{\beta}_+ + \ddot{\beta}_+^2 - 24\ddot{\beta}_+ \dot{\beta}_+^2 + 12\dot{\beta}_+^4, \\ B_{22} &= \sqrt{3}(\ddot{\beta}_- - 24\ddot{\beta}_- \dot{\beta}_-^2 - 8\ddot{\beta}_- \dot{\beta}_+^2 - 16\dot{\beta}_- \ddot{\beta}_+ \dot{\beta}_+) + 2\ddot{\beta}_- \dot{\beta}_- - \ddot{\beta}_-^2 \\ &\quad + 16\ddot{\beta}_- \dot{\beta}_- \dot{\beta}_+ - 12\dot{\beta}_-^4 + 8\dot{\beta}_-^2 \ddot{\beta}_+ - 24\dot{\beta}_-^2 \dot{\beta}_+^2 - \ddot{\beta}_+ \\ &\quad + 2\ddot{\beta}_+ \dot{\beta}_+ - \ddot{\beta}_+^2 + 24\ddot{\beta}_+ \dot{\beta}_+^2 - 12\dot{\beta}_+^4, \\ B_{33} &= 2\ddot{\beta}_- \dot{\beta}_- - \ddot{\beta}_-^2 + 32\ddot{\beta}_- \dot{\beta}_- \dot{\beta}_+ - 12\dot{\beta}_-^4 - 16\dot{\beta}_-^2 \ddot{\beta}_+ - 24\dot{\beta}_-^2 \dot{\beta}_+^2 \\ &\quad + 2\ddot{\beta}_+ \dot{\beta}_+ + 2\ddot{\beta}_+ \dot{\beta}_+ - \ddot{\beta}_+^2 - 48\ddot{\beta}_+ \dot{\beta}_+^2 - 12\dot{\beta}_+^4. \end{aligned}$$

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*“When you have read these hastily
scrawled pages you may guess, though
never fully realize, why it is that I must
have forgetfulness or death.”*

— H. P. Lovecraft, “Dagon”

